Aspen Engineering Suite 2004.1

Aspen Plus

Input Language Guide

aspentech
driving process profitability

Who Should Read this Guide

This manual is a reference for users who need to understand the input language Aspen Plus uses to communicate between the GUI and Engine, and for users who need to understand the variables Aspen Plus uses for sequential modular simulations.

The input language is contained in .INP files which you can also export from the Aspen Plus GUI. Advanced users may also write their own input files.

The variables are used in blocks such as Calculator, Design Spec, and Sensitivity where model variable values may be read or manipulated by other models.

Contents

Introducing the Input Language Guide

The *Aspen Plus Input Language Guide* lists and describes the input language for all Aspen Plus capabilities except costing. This guide supplements the documentation set for Aspen Plus, and is intended for experienced Aspen Plus users who choose not to use the Aspen Plus graphical user interface for certain modeling projects.

This guide also lists the variables for each block accessible through sequential modular flowsheeting manipulations such as Calculator blocks and Design Specs.

1 Aspen Plus Input Language

This chapter describes:

- Input language elements.
- Rules for using input language.
- Rules for writing an input language file.

Input Language Elements

The Aspen Plus input language consists of:

- Paragraphs
- Sentences
- Data entry

Corresponding to this hierarchy are three levels of keywords: primary, secondary, and tertiary. In addition, an input file can contain comments and inline FORTRAN statements.

Paragraphs

A paragraph is a logical group of input data, such as the data describing a stream or a unit operation block. All paragraphs begin with a primary keyword. The following paragraph describes a unit operation block that models a reactor. The primary keyword is BLOCK:

```
BLOCK   REACT   RSTOIC
PARAM   TEMP=400   PRES=-15
STOIC   1   MIXED   BZ   -1 / H2   -3 / CH   1
CONV    1   MIXED   BZ   0.998
```

Sentences

A sentence is a free format string of entries beginning with a secondary keyword. The paragraph in the previous example has three sentences: PARAM, STOIC, and CONV. The PARAM sentence contains data concerning the reactor outlet conditions. The STOIC sentence describes reaction stoichiometry, and the CONV sentence describes the conversion of benzene.

Data Entry

You can enter sentence data either by position or by tertiary keyword. Sentence data entered by tertiary keywords can appear in any order. The PARAM sentence in the previous example uses the TEMP and PRES tertiary keywords for data entry. The STOIC and CONV sentences use positional input.

A data entry can be a number or a character string. When entering a number, use any valid FORTRAN constant, either integer or real. Aspen Plus automatically makes the appropriate conversion. Character strings are made up of the following characters:

A-Z 0-9 $, : + – _

The first character must be alphabetic or numeric. The character string must be enclosed in quotes, if the following special characters are used:

(Blank) ; / = * . & ( ) [ ] { } < >

The following example shows input language for the RSTOIC model:

```
BLOCK    blockid    RSTOIC
PARAM    keyword=value
```

Keywords:

TEMP PRES VFRAC DUTY

Optional keywords*:*

NPHASE PHASE SERIES MAXIT TOL

```
STOIC    reacno    ssid    cid    coef  /  cid    coef  /  . . .
EXTENT   reacno    extent  /  . . .
CONV     reacno    ssid    key-cid    conv  /  . . .
COMP-ATTR    entryno    ssid    cattrname    (value-list)
SUBS-ATTR    entryno    ssid    psdid    (value-list)
```

Rules for Using Aspen Plus Input Language

You must observe the following rules when using this guide:

- Enter capitalized names and keywords, verbatim. Lowercase letters indicate user-supplied quantities.
- Brackets [ ] indicate that a positional keyword is optional. Tertiary keywords are listed as either required or optional.
- Ellipsis dots (**. . .**) indicate repeated entries**.**
- Braces { } indicate that you are to enter one of the options enclosed within the braces.
- Substitute MOLE, MASS, or STDVOL for the lowercase word *basis*, depending on whether your data are on a mole, mass, or standard-liquid-volume basis.

The following table describes rules that relate to lowercase words:

If a lowercase word ends in	You can enter
no	An integer value that Aspen Plus uses as an identifier
name or type	A name selected from a specified list of built-in names (for example, the name of an Aspen Plus model)
list	A list of entries
id	A character string of up to eight characters

Aspen Plus uses the character string as an identifier (ID). You can use any character string. You cannot use the dollar sign as the first character, because it is reserved for system-generated IDs. The following list contains abbreviations for IDs used in this manual:

ID	Description
cid	Component ID
gid	UNIFAC group ID
optid	Optimization ID
pcid	Pseudocomponent ID
seqid	Sequence ID
sid	Stream ID
specid	Design-spec ID

Rules for Writing an Aspen Plus Input File

Follow these rules when writing an input file:

- The length of an input line is 80 characters.
- Blanks are used to separate entries. When the following special characters are used, blanks are not needed: semicolon, slash (/), left or right parenthesis, left or right square bracket, equal sign, ampersand, and single or double quotes.
- Primary keywords start in column one. Secondary keywords can start in any column except column one.
- Paragraphs can be entered in any order.
- An ampersand (&) is used to continue a sentence on more than one line. Place the ampersand at the end of the line to be continued. You do not need the ampersand when the line to be continued ends in a slash, or when a quoted string is continued on more than one line. The second and subsequent lines must have blanks in column one.
- Anything after a semicolon (;), and on the same line, is treated as a comment.
- The names ALL, NONE, and MISSING are reserved names. They should not be used for any block IDs, component IDs, and so on.

See the *Aspen Plus User Guide* for rules relating to inline FORTRAN.

2 Running Aspen Plus

Aspen Plus simulations can run both interactively and non-interactively, using input language. In the interactive environment you can communicate directly with Aspen Plus to perform actions. Actions include executing part or all of the simulation, viewing simulation results, and making input changes. In the non-interactive environment, you cannot communicate with Aspen Plus. The non-interactive environment only allows you to enter Aspen Plus commands; it lets the simulation engine complete the work.

This chapter describes the ASPEN run command. It also includes information about using interactive simulation capabilities.

The ASPEN Run Command

The ASPEN run command invokes Aspen Plus to process your input file and perform the specified simulation. You must enter the ASPEN command and its qualifiers in lowercase for UNIX operating systems, unless otherwise specified. For Windows operating systems, the ASPEN command is not case sensitive. This section describes only the basic usage of the ASPEN command.

Operating System	Command
Windows	**ASPEN** ***input_file [runid]***

Where:

input_file	=	A file written in Aspen Plus input language that defines theproblem to be simulated. The default file type is .inp. You do not need to include it in the command line.
runid	=	The identifier for the current simulation for single ID runs. For EDIT runs with two IDs, runid is the identifier for the previous simulation program to be edited. (See Chapter 47.)
newrunid	=	The identifier used when you want to make an EDIT run in OpenVMS and UNIX operating systems. (See Chapter 47.)

The runid parameter must always be specified for EDIT runs. For non-EDIT runs, if the runid is not specified, the runid defaults to the input_file value, stripped of the directory specification. The runid is limited to eight characters, and Aspen Plus truncates it if necessary. It is used to generate files needed during the simulation. Files generated by Aspen Plus will have the runid as the file name, followed by a three-character file type descriptor.

For information about advanced use of the ASPEN command, run it with no input file specified.

Choosing the Simulation Environment

To run the simulation interactively, you must include the following paragraph in your Aspen Plus input file:

```
SIMULATE INTERACTIVE=YES
```

Otherwise Aspen Plus assumes that your simulation runs non-interactively.

Working in the Interactive Environment

When running Aspen Plus interactively, you can communicate with Aspen Plus by:

- Using interactive commands to perform actions (for example, executing part or all of the simulation or displaying results). You enter commands at the Aspen Plus prompt (A+>). See Interactive Commands, this chapter, for more information.
- Viewing simulation results and making input changes in your computer system's text editor. See Simulation Results, this chapter, for more information.

Interactive Commands

You can use the interactive commands in Table 2.1. To get a menu of all available commands, type a question mark (?) at the Aspen Plus prompt. To get online help on these commands, type HELP. Descriptions of the commands follow in Table 2.2.

Table 2.1 Interactive Commands

Command	Description
ADVENT	Generates interface information for ADVENT.
CANCEL STOP	Cancels one or all stop points. See CANCEL STOP Command, this chapter.
DISPLAY	Displays current results of the simulation. For example, you can display blocks, streams, material, and energy balance. See DISPLAY Command, this chapter.
EDIT	Lets you view or modify specifications for the simulation. See EDIT Command, this chapter.
END	Ends the simulation. The problem data file and the input file are updated with any changes you have made. The END and EXIT commands are synonymous. Use the QUIT command to terminate the simulation without updating the problem data file and input file, and without incorporating your changes to the simulation.
EXIT	Ends the simulation. The problem data file and the input file are updated with any changes you have made. The EXIT and END commands are synonymous. Use the QUIT command to terminate the simulation without updating the problem data file and input file, and without incorporating your changes to the simulation.
FEDIT	Invokes your computer system editor so that you can edit a file. FEDIT can be useful if you need to view another file during a simulation. For example, you may want to view the input file for another problem or case. Any changes you make to the file do not affect the simulation. You cannot use FEDIT to view the history or report file for the current simulation. Use the DISPLAY command to view these files.

continued

Table 2.1 Interactive Commands (continued)

Command	Description
GO	Begins or continues execution of the simulation. The simulation will proceed until one of the following occurs: • A stop point is encountered. • You press the hot key. • The end of the calculation sequence is reached. If you are at the end of the calculation sequence (all blocks have been executed), GO generates a report.
HELP	Invokes the interactive simulation help facility to display information about an interactive command or topic
MOVETO	Moves to another block in the calculation sequence. The block that you move to is the first block that is executed when you type GO, NEXT, or RUN. See MOVETO Command, this chapter.
NEWNAME	Creates a new case, opens a new file; closes the current report file, ADVENT interface file, summary file, and plot file. You can specify a report title that appears at the top of every page in the report, replacing the title specified in the TITLE paragraph in the input file. The new case name can be up to 8 characters long. The report title can be up to 64 characters long.
NEXT	Executes the next block in the calculation sequence.
PRINT	Prints the results you reviewed with the most recent DISPLAY command. You can specify printer options (such as print queue) in the Aspen Plus initialization file, ap.ini. You can override the options from the initialization file by specifying the operating system print command as an option in the PRINT command. If your computer system requires that you specify print options after the file name, use an asterisk (*) for the file name.
QUIT	Terminates the simulation. The problem data file and the input file are not updated with any changes you have made. Use the END or EXIT commands to end the simulation and update the problem data file and input file, incorporating changes you have made.
REINIT	Reinitializes unit operation blocks, convergence blocks, regression blocks, or streams to their default values. See REINIT Command, this chapter.
REPORT	Generates an Aspen Plus report file, summary file, or XML file. You can also provide a report heading that appears in the table of contents for the report. The heading can be up to 64 characters long. You can use the DISPLAY REPORT command to view the report. See REPORT Command, this chapter.
RUN	Continues the simulation ignoring all stop points. Aspen Plus completes the simulation, generates a report, and exits. You can regain control at any point during the simulation by pressing the hot key.
SHOW	Shows specified information about the simulation, such as the list of blocks or the calculation sequence. The information is written to your terminal. Use the DISPLAY command to view results of the simulation. See SHOW Command, this chapter.
SPAWN	Creates an operating system shell (subprocess), from which you can execute operating system commands. See SPAWN Command, this chapter.
STOP	Sets a stop point. You can identify the stop point as being either before or after a block, or after a warning or error has occurred. A stop point after a convergence block causes the simulation to stop at the beginning of each iteration of the block, and after the block has terminated. Aspen Plus assigns a number to each stop point. (The first stop you enter is stop 1.) You can display a list of stop points with the SHOW STOPS command. To display stop points in the calculation sequence, use the SHOW SEQUENCE command.

continued

Table 2.1 Interactive Commands (continued)

Command	Description
SYNCEO	Synchronize the equation-oriented simulation based on the current sequential modular simulation.
TOEO	Start accepting commands for equation-oriented simulation. See the *OOMF Script Language Reference Manual* for more information. To return to the sequential modular command processor, type QUIT.

Table 2.2 Interactive Command Characteristics

Characteristics	Description
Case Sensitivity	Aspen Plus is not case sensitive. You can type your commands in either uppercase or lowercase.
Partial Matching of Commands	You can abbreviate interactive commands. You only need to type enough letters to make the command unique. If the command you have typed is not unique, Aspen Plus gives you a list of the commands that begin with the letters you typed. For example, if you type the command S and there is more than one command that starts with S, Aspen Plus lists all commands that start with S.
Incomplete Commands	If you do not complete a command, or if a word cannot be recognized, Aspen Plus recognizes as much of the command as possible and gives you a menu of items to complete the command. For example, if you enter the command DISPLAY, Aspen Plus displays the list of items that can be displayed. If you then type the item BLOCK, Aspen Plus gives you a list of blocks. At each point, the prompt includes as much of the command as is complete. You can build up a command one word at a time, with Aspen Plus prompting you for each word to complete the command.
Canceling Commands	When building a command one item at a time (see Incomplete Commands), you can use the less than character (<) to cancel one item of the command. For example, if you enter the command DISPLAY BLOCK, Aspen Plus displays a list of blocks . It also displays the partial command DISPLAY BLOCK in the prompt. If you want to display a stream instead, you can enter < to cancel BLOCK. Aspen Plus displays the partial command DISPLAY in the prompt. You can then type STREAM to display a stream.
Viewing Results	When you use the DISPLAY command to view results, Aspen Plus writes the results to a temporary file. Then it invokes the text editor for your computer system to view the file. You can use all the features of your editor, including searching for text strings, scrolling, and writing the file to disk for later use. When you are finished viewing the results, quit from the editor (leave the editor without updating the file). After leaving the editor, you can use the PRINT command (at the Aspen Plus prompt) to print the file you just viewed.
Making Input Changes	When you use the EDIT INPUT command to make changes, Aspen Plus invokes the text editor for your computer system with your input file. When you use the EDIT BLOCK or EDIT STREAM commands, Aspen Plus extracts the appropriate paragraph from your input file and invokes your editor containing that paragraph. When you are finished making your changes, exit from the editor (leave the editor and update the file). If you quit from the editor, or if you exit without making changes to the file, no change is made to the simulation. When you edit the input file, Aspen Plus detects which paragraphs have been added, modified, or deleted, and updates the simulation accordingly. (Table 2.3 summarizes the paragraphs that can be added, modified, or deleted.)

continued

Table 2.2 Interactive Command Characteristics (continued)

Characteristics	Description
Adding and Modifying Input	You can add most Aspen Plus paragraphs to your input file. You can add blocks to your flowsheet by adding a BLOCK sentence to the FLOWSHEET paragraph and adding the BLOCK paragraph. You cannot add paragraphs related to properties. (See Table 2.3 for a list of the paragraphs you can add, modify, or delete in interactive mode.) Most paragraphs that can be added can also be modified. An important exception is the PROP-SET paragraph. You can add a PROP-SET paragraph, but you cannot modify it.
Deleting	To delete blocks from the simulation, delete the BLOCK paragraph from your input file and delete the corresponding BLOCK sentence from the FLOWSHEET paragraph. You can delete DESIGN-SPEC paragraphs, CONVERGENCE blocks, and many other items the same way. Some paragraphs can be added and modified but not deleted, such as paragraphs for report options. To delete the effect of these paragraphs, you must modify the paragraph so that it has default values. **Note:** Do not use the Aspen Plus DELETE paragraph in your input file.
Input Errors	If you make errors when modifying the input, Aspen Plus writes the error messages to the terminal. Then Aspen Plus returns to your input file, so you can correct the errors. The messages are also written to the top of the input file. If you quit from the editor or exit without fixing the errors, Aspen Plus does not allow you to continue the simulation.
Hot Key	You can regain control of the simulation at any point by pressing the hot key. Aspen Plus completes the block currently executing, then returns to the Aspen Plus prompt. If the current block is RADFRAC, MULTIFRAC, PETROFRAC, or EXTRACT, Aspen Plus stops at the end of the current iteration and returns to the interactive prompt. If the current block is RPLUG, RBATCH, or PRES-RELIEF, Aspen Plus stops at the end of the current iteration of the current integration step.

The hot key is Ctrl+BREAK or Ctrl+C.

CANCEL STOP Command

When you use the STOP command to set a stop point, Aspen Plus assigns a number to the stop point. You must use this number to cancel that stop point. You can review the stop numbers by using the SHOW STOPS command. Stops are also shown in the calculation sequence, which you can display using the SHOW SEQUENCE command. When you cancel a stop point, Aspen Plus renumbers all remaining stop points.

If you choose this option	Aspen Plus cancels
stopno	Stop *stopno*
ALL	All stop points

DISPLAY Command

The following table describes the options you can choose when you use the DISPLAY command:

If you choose this option	Aspen Plus displays
BALANCE	Material and energy balances for the flowsheet
BBLOCK *balanceid*	Balance block *balanceid*
BLOCK *blockid*	Unit operations block *blockid*
CALCULATOR *cblockid*	CALCULATOR block *cblockid*
CONNSTREAM *blockid*	Connecting streams for block *blockid*
CONSTRAINT *conid*	Constraint *conid*
CONVERGENCE *cvblockid*	Convergence block *cvblockid*
DESIGN-SPEC *specid*	DESIGN-SPEC *specid*
HISTORY	History file
OPTIMIZATION *oblockid*	Optimization block *oblockid*
PRES-RELIEF *pblockid*	Pressure relief block *pblockid*
PROP-TABLE *tableid*	PROP-TABLE *tableid*
REGRESSION *rblockid*	Regression block *rblockid*
REPORT	Report file
SENSITIVITY *sblockid*	Sensitivity block *sblockid*
STATUS	Convergence status summary
STREAMS *sid-list*	The listed streams. Enter ALL for *sid-list* to display all streams.
TOC	Table of contents for report
TRANSFER *tblockid*	Transfer block *tblockid*

The DISPLAY command allows you to view results using the default text editor for your computer system. (You can change the default text editors for interactive Aspen Plus in the initialization file, ap.ini.)

EDIT Command

You can edit an individual block paragraph, an individual stream paragraph, or the entire input file. Aspen Plus invokes your computer system's editor to make your changes to the paragraph or the input file. If you quit from your editor (without saving your changes), no changes are made to the simulation. When you exit the editor (saving your changes), Aspen Plus updates the simulation problem. (You can change the default text editors for interactive Aspen Plus in the initialization file, ap.ini.)

When you edit the input file, Aspen Plus detects which paragraphs you have added, modified, or deleted, and updates the simulation accordingly. The paragraphs that can be added, modified, or deleted during an Aspen Plus interactive simulation appear in Table 2.2.

If you choose this option	Aspen Plus edits
INPUT	Input file
BLOCK *blockid*	Block paragraph for block *blockid*
STREAM *sid*	Stream paragraph for stream *sid*

MOVETO Command

The following table describes the options you can choose when you use the MOVETO command:

If you choose this option	Aspen Plus moves to
BBLOCK *balanceid*	Balance block *balanceid*
BLOCK *blockid*	Unit operations block *blockid*
CALCULATOR *cblockid*	CALCULATOR block *cblockid*
CONVERGENCE *cvblockid*	Convergence block *cvblockid*
END	End of sequence (after the last block)
PRES-RELIEF *pblockid*	Pressure relief block *pblockid*
REGRESSION *rblockid*	Regression block *rblockid*
SENSITIVITY *sblockid*	Sensitivity block *sblockid*
START	First block in sequence
TRANSFER *tblockid*	Transfer block *tblockid*

REINIT Command

Reinitializing a unit operation block, regression block, or a convergence block causes Aspen Plus to use the initial guess you supplied in the input file. Or Aspen Plus generates a new initial guess, rather than restarting from the results of the last block execution. Reinitializing a stream resets the stream composition flow rate and conditions to those specified in the STREAM paragraph in the input file. If you do not provide a STREAM paragraph for a stream, the stream is reset to a flow rate of zero.

If you choose this option	Aspen Plus reinitializes
ALL	All unit operation blocks, convergence blocks, and streams
BLOCKS *block-list*	The listed unit operation blocks. Enter ALL for *block-list* to reinitialize all unit operation blocks.
CONVERGENCE *cvblock-list*	The listed convergence blocks. Enter ALL for *cvblock-list* to reinitialize all convergence blocks.
REGRESSION *rblock-list*	The listed regression blocks. Enter ALL for *rblock-list* to reinitialize all regression blocks.
STREAMS *sid-list*	The listed streams. Enter ALL for *sid-list* to reinitialize all streams.

REPORT Command

The following table describes the options you can choose when you use the REPORT command:

If you choose this option	Aspen Plus reports the results of the run in
SUMMARY	A summary file
REPORT	A report file
BOTH	Both a summary file and a report file
XML	A summary file in XML format

SHOW Command

The following table describes the options you can choose when you use the SHOW command:

If you choose this option	Aspen Plus shows
BLOCKS	All blocks (unit operation, convergence) and their status
CASES	Name and status of all cases created with the NEWNAME command
FLOWSHEET	Flowsheet connectivity by blocks
SEQUENCE	Calculation sequence
STOPS	Stop points you have set
STREAMS	All streams with source and destination

SPAWN Command

The SPAWN command creates a new system process. You can use it, for example, to read your mail without exiting from the simulation. You can also create a shell to print a report file. First you must use the REPORT command to generate the report and the NEWNAME command to close the report.

You can specify an optional operating system command that executes immediately. If you do not enter an operating system command as an option in the shell command, you must enter the appropriate command for your computer and operating system to return to Aspen Plus:

For this operating system	Use this command to return to Aspen Plus
Windows	**EXIT**

Simulation Results

Aspen Plus produces the following files:

This file	Contains
HISTORY	Information about the status of your simulation run
REPORT	Simulation results

When you issue a command to display results, Aspen Plus writes the results to a temporary file and places you in your editor viewing that file. You can scroll, search for strings, or use any of the other features of your editor. Similarly, when you issue a command to change the input specifications, Aspen Plus places you in your editor with your input file, or part of your input file.

HISTORY File

Whenever you use the EDIT command to change your input specifications, the changed paragraphs are written to the history file. You can browse through the history file at any point during an interactive run, using the command DISPLAY HISTORY.

REPORT File

When you use the REPORT command to generate a report, the report is written to two files. The table of contents is written to one file, and the actual report to another file. You can view the table of contents with the command DISPLAY TOC. You can view the report with the command DISPLAY REPORT.

If you use the REPORT command more than once in a simulation, Aspen Plus, by default, writes all reports to the same file. The second report is appended to the first as an additional case, and so on. You can specify an optional heading for a case in the REPORT command. This heading will be written into the table of contents for reports after the first report. Alternatively, you can use the NEWNAME command to:

- Close the current report file, ADVENT interface file, plot file, and summary file.
- Open new files with different names.

You can also specify a title in the NEWNAME command. Aspen Plus writes this title to the top of every page of the report, replacing the title specified in the TITLE paragraph of your input file.

Interactive Changes and Input File

The following table describes what happens to the input specifications when you use these commands:

If you enter	Aspen Plus does the following to your input file
EDIT	Updates a copy of it
END	Adds your changes
EXIT	Adds your changes
QUIT	Does not add changes

Aspen Plus always makes a copy of your original input file. The copy is called runid.in0.

Table 2.3 lists the Aspen Plus paragraphs that can appear in an Aspen Plus input file. The table indicates whether they can be added, modified, or deleted in an interactive simulation:

Table 2.3 Aspen Plus Paragraphs for Interactive Runs

Paragraph	Added	Modified	Deleted
ADA-REPORT	Yes	Yes	No
ADVENT	Yes	Yes	No
BALANCE	Yes	Yes	No
BLOCK	Yes	Yes	Yes
BLOCK-REPORT	Yes	Yes	No
CALCULATOR	Yes	Yes	Yes
CASE-STUDY	Yes	Yes	Yes
COMP-GROUP	Yes	Yes	No
CONSTRAINT	Yes	Yes	Yes
CONVERGENCE	Yes	Yes	Yes
CONV-OPTIONS	Yes	Yes	No
CONV-ORDER	Yes	Yes	Yes
DATA-SET	Yes	Yes	Yes
DEBUG	Yes	Yes	No
DEF-STREAMS	Yes	No	No
DEF-STREAM-ATTR	Yes	No	No
DEF-STREAM-CLASS	Yes	No	No
DEF-SUBS	Yes	No	No
DEF-SUBS-ATTR	Yes	No	No
DEF-SUBS-CLASS	Yes	No	No
DELETE	Yes	Yes	No
DESCRIPTION	Yes	Yes	No
DESIGN-SPEC	Yes	Yes	Yes
DIAGNOSTICS	Yes	Yes	No
FLOWSHEET	Yes	Yes	Yes
FLOWSHEET-REPORT	Yes	Yes	No
IN-UNITS	Yes	Yes	No
NOSIMULATE	Yes	Yes	No
OPTIMIZATION	Yes	Yes	Yes
OUT-UNITS	Yes	Yes	No
PLOT-OPTIONS	Yes	Yes	No
PRES-RELIEF	Yes	Yes	Yes
PROFILE-DATA	Yes	Yes	Yes
PROPERTY-REPORT	Yes	Yes	No
PROP-SET	Yes	No	No
PROP-TABLE	Yes	Yes	Yes
REACTIONS	Yes	Yes	Yes
REGRESSION	Yes	Yes	Yes

continued

Table 2.3 Aspen Plus Paragraphs for Interactive Runs (continued)

Paragraph	Added	Modified	Deleted
REPORT	Yes	Yes	No
REPORT-SCALE	Yes	Yes	Yes
RUN-CONTROL	Yes	Yes	No
SENSITIVITY	Yes	Yes	Yes
SEQUENCE	Yes	Yes	Yes
SIM-OPTIONS	Yes	Yes	No
STREAM	Yes	Yes	Yes
STREAM-REPORT	Yes	Yes	No
SUMMARY	Yes	Yes	No
SYS-OPTIONS	Yes	Yes	No
TEAR	Yes	Yes	Yes
TITLE	Yes	Yes	No
TRANSFER	Yes	Yes	Yes
USER-PROPERTY	Yes	Yes	No

3 Units

This chapter describes the input language for specifying units in Aspen Plus. Aspen Plus has three built-in units sets:

- English Engineering (ENG).
- International System (SI).
- Metric Engineering (MET).

The English Engineering set is the default. You can override the built-in units for individual units type. You can also create your own units for an existing physical quantity type with the CUSTOM-UOM paragraph.

Specifying Units

You can specify input units globally, for a paragraph, or for an individual data item:

To specify	You must
Input units globally	Use an IN-UNITS paragraph
Input units for data in a particular paragraph	Use an IN-UNITS sentence at the beginning of a paragraph
A units option for an individual data value	Follow the value by the desired option, enclosed in [ ], { }, or < >

You can use the OUT-UNITS paragraph to specify units for the report file (see Chapter 46). If no OUT-UNITS paragraph is given, Aspen Plus uses the IN-UNITS global specification. All values printed in the history file are in SI units (see Chapter 45).

Input Language for IN-UNITS

```
IN-UNITS    set    keyword=option
OUT-UNITS   set    keyword=option
```

Input Language Description for IN-UNITS

set ..... ENG, SI, or MET (Default=ENG)

keyword..... Units keyword. (See Table 3.1.)

option ..... Units option. (See Table 3.1.) This specification overrides the corresponding units option contained in the specified set.

Table 3.1 Units Options

See the following table for explanations of some units symbols.

Type of Units	SI Set	ENG Set	MET Set	Other Units Options
ANGLE	RAD	DEG	DEG	
AREA	SQM	SQFT	SQM	SQCM, SQIN, SQMILE, SQMM
AREA-PRICE	$/SQM	$/SQFT	$/SQM	$/SQCM, $/SQIN, $/SQMILE, $/SQMM
AREA-USAGE	SQM/SEC	SQFT/HR	SQM/HR	SQM/DAY, SQM/YEAR
BOND-WORK-IN	J/KG	KWHR/TON	KWHR/TON	KJ/KG
CHROM-VEL	M/SEC	FT/SEC	CM/HR	
COMPOSITION	MOL-FR	MOL-FR	MOL-FR	MASS-FR
CONTENTS	FRACTION	PERCENT	FRACTION	PPM
COST-RATE	$/SEC	$/HR	$/HR	$/MIN, $/DAY, $/YEAR, K$/HR, K$/DAY, K$/YEAR, MM$/DAY, MM$/YEAR
CURRENT	AMP	AMP	AMP	MAMP
DELTA-T	K	F	K	C, R, DELTA-K, DELTA-F, DELTA-C, DELTA-R
DENSITY	KG/CUM	LB/CUFT	GM/CC	LB/GAL, GM/CUM, GM/ML, LB/BBL
DIFFUSIVITY	SQM/SEC	SQFT/HR	SQCM/SEC	CS
DIMENSIONLES	UNITLESS	UNITLESS	UNITLESS	UNTLESS, UNITLES
DIPOLEMOMENT	(J*CUM)**.5	(BTU*CUFT)**.5	DEBYE	(KJ*CUM)**.5
ELEC-POWER	WATT	KW	KW	

Type of Units	SI Set	ENG Set	MET Set	Other Units Options
ELEC-PRICE	$/J	$/KWHR	$/KWHR	
ENERGY	J	BTU	CAL	KCAL, KWHR, FT-LBF, GJ, KJ, N-M, MJ, MCAL, GCAL, MBTU, MMBTU, HP-HR
ENERGY-PRICE	$/J	$/BTU	$/CAL	$/KCAL, $/KWHR, $/FT-LBF, $/GCAL, $/MMBTU, $/HP-HR, $/MBTU, $/KJ, $/MJ, $/GJ, $/N-M, $/MCAL
ENERGY-VOL	CUM/J	BBL/BTU	CUM/J	BBL/MMBTU
ENTHALPY	J/KMOL	BTU/LBMOL	CAL/MOL	J/KG, BTU/LB, CAL/GM, MBTU/LBMOL
ENTHALPY-CYC	WATT/CYCLE	BTU/CYCLE	CAL/CYCLE	J/CYCLE, GJ/CYCLE, KCAL/CYCLE, MMKCAL/CYCLE, MMBTU/CYCLE, MMKCAL/CYCLE, MMBTU/CYCLE, PCU/CYCLE, MMPCU/CYCLE, KJ/CYCLE, KW/CYCLE, GCAL/CYCLE
ENTHALPY-FLO	WATT	BTU/HR	CAL/SEC	J/SEC, GJ/HR, KCAL/HR, MMKCAL/HR, MMBTU/HR, MMKCAL/DAY, MMBTU/DAY, PCU/HR, MMPCU/HR, KJ/SEC, KW, MW, GW, MJ/HR, GCAL/HR, MBTU/HR, GCAL/DAY
ENTHALPY-OPR	WATT/CYCLE	BTU/OP-HR	CAL/OP-SEC	J/OP-SEC, GJ/OP-HR, KCAL/OP-HR, MMKCAL/OP-HR, MMBTU/OP-HR, MMKCAL/OP-DAY, MMBTU/OP-DAY, PCU/OP-HR, MMPCU/OP-HR, KJ/OP-SEC, KW/CYCLE, GCAL/OP-HR, GCAL/OP-DAY
ENTROPY	J/KMOL-K	BTU/LBMOL-R	CAL/MOL-K	J/KG-K, BTU/LB-R, CAL/GM-K, MJ/KMOL-K, KCAL/KMOL-K, GCAL/KMOL-K, MBTU/LBMOL-R
F-FACTOR	(KG-CUM)**.5/SEC	(LB-CUFT)**.5/HR	(GM-L)**.5/MIN	(LB-GAL)**.5/MIN
FILTER-RESIS	1/METER	1/FT	1/METER	1/CM, 1/IN
FISCAL	$	$	$	
FLOW	KG/SEC	LB/HR	KG/HR	LB/SEC, MLB/HR, TONS/DAY, MCFH, TONNE/HR, LB/DAY, KG/DAY, TONS/HR, KG/MIN, KG/YEAR, GM/MIN, GM/HR, GM/DAY, MGM/HR, GGM/HR, MGM/DAY, GGM/DAY, LB/MIN, MMLB/HR, MLB/DAY, MMLB/DAY, LB/YEAR, MLB/YEAR, MMLB/YEAR, TONS/MIN, MTONS/YEAR, MMTONS/YEAR, L-TONS/MIN, L-TONS/HR, L-TONS/DAY, ML-TONS/YEAR, MML-TONS/YEAR, KTONNE/YEAR
FLUX	CUM/SQM-SEC	CUFT/SQFT-SEC	L/SQM-SEC	L/SQM-HR, GAL/SQFT-MIN
FLUX-HEAT-AR	WATT/SQM	BTU/HR-SQFT	CAL/SEC-SQM	J/SEC-SQM, MMBTU/HR-SQFT, KW/SQM
FLUX-MOLE	KMOL/SQM-S	LBMOL/SQFT-HR	KMOL/SQM-HR	LBMOL/SQFT-S, MOL/SQCM-S
FORCE	NEWTON	LBF	DYNE	
FREQUENCY	HZ	RPM	RPM	RAD/SEC, RPS, KRPM, MMRPM, RPH
HEAD	J/KG	FT-LBF/LB	M-KGF/KG	SQM/SQSEC, INCH, FT, METER, KJ/KG, KM-KGF/KG, MFT, MJ/KG, MFT-LBF/LB, FT-HEAD, METER-HEAD, INCH-HEAD
HEAT	J	BTU	CAL	KCAL, MMKCAL, MMBTU, PCU, MMPCU, KJ, GJ, N-M, MJ, MCAL, GCAL, MBTU, KW-HR
HEAT-FLUX	WATT/M	BTU/HR-FT	CAL/SEC-M	J/SEC-M, MMBTU/HR-FT
HEAT-RATE-V	WATT/CUM	BTU/HR-CUFT	CAL/SEC-CUM	J/SEC-CUM, MMBTU/HR-CUFT, GJ/HR-CUM
HEAT-TRANS-C	WATT/SQM-K	BTU/HR-SQFT-R	CAL/SEC-SQCM-K	KCAL/SEC-SQM-K, KCAL/HR-SQM-K, PCU/HR-SQFT-K, KW/SQM-K, J/SEC-SQM-K, KJ/SEC-SQM-K, MMBTU/HR-SQFT-R, KJ/SEC-SQM-C, MJ/SEC-SQM-K, MJ/SEC-SQM-C, GJ/HR-SQM-K, GJ/HR-SQM-C, KCAL/HR-SQM-C, BTU/HR-SQFT-F
INVERSE-AREA	1/SQM	1/SQFT	1/SQM	

Type of Units	SI Set	ENG Set	MET Set	Other Units Options
INVERSE-HT-C	SQM-K/WATT	HR-SQFT-R/BTU	SEC-SQCM-K/CAL	SEC-SQM-K/KCAL, HR-SQM-K/KCAL, HR-SQFT-K/PCU, SQM-K/KW, SEC-SQM-K/J, SEC-SQM-K/KJ
INVERSE-LENG	1/M	1/FT	1/CM	1/IN, 1/MM
INVERSE-PRES	SQM/N	1/PSI	1/ATM	SQFT/LBF, 1/BAR, 1/TORR, 1/IN-WATER, SQCM/KG, 1/MMHG, 1/KPA, 1/MM-WATER
INVERSE-TEMP	1/K	1/R	1/K	
INVERSE-TIME	1/SEC	1/HR	1/HR	1/MIN, 1/DAY, 1/YEAR
ITEM-PRICE	$/ITEM	$/ITEM	$/ITEM	
LENGTH	METER	FT	METER	CM, IN, MU, MM, MILE, KM, ANGSTROM, MFT
LN-INV-TIME	LN(1/SEC)	LN(1/HR)	LN(1/HR)	LN(1/MIN)
MASS	KG	LB	KG	GM, TON, MLB, TONNE, L-TON, MMLB
MASS-CONC	KG/CUM	LB/CUFT	GM/L	GM/CC, MG/L, MG/CC
MASS-CYCL	KG/CYCLE	LB/CYCLE	KG/CYCLE	LB/CYCLE, MLB/CYCLE, TONS/CYCLE, GM/CYCLE, TONNE/CYCLE, LB/CYCLE, KG/CYCLE, TONS/CYCLE, TONS/CYCLE
MASS-DENSITY	KG/CUM	LB/CUFT	GM/CC	LB/GAL, GM/CUM, GM/ML
MASS-ENTHALP	J/KG	BTU/LB	CAL/GM	KCAL/KG, MMKCAL/KG, MMBTU/LB, PCU/LB, MMPCU/LB, KJ/KG, MJ/KG, GCAL/KG, MBTU/LB
MASS-ENTROPY	J/KG-K	BTU/LB-R	CAL/GM-K	KCAL/KG-K, KJ/KG-K, MJ/KG-K, GCAL/KG-K, MBTU/LB-R
MASS-FLOW	KG/SEC	LB/HR	KG/HR	LB/SEC, MLB/HR, TONS/DAY, GM/SEC, TONNE/HR, LB/DAY, KG/DAY, TONS/YEAR, TONS/HR, TONNE/DAY, TONNE/YEAR, KG/MIN, KG/YEAR, GM/MIN, GM/HR, GM/DAY, MGM/HR, GGM/HR, MGM/DAY, GGM/DAY, LB/MIN, MMLB/HR, MLB/DAY, MMLB/DAY, LB/YEAR, MLB/YEAR, MMLB/YEAR, TONS/MIN, MTONS/YEAR, MMTONS/YEAR, L-TONS/MIN, L-TONS/HR, L-TONS/DAY, ML-TONS/YEAR, MML-TONS/YEAR, KTONNE/YEAR
MASS-FLUX	KG/SQM-S	LB/SQFT-HR	KG/SQM-HR	LB/SQFT-S, GM/SQCM-S, KG/SQCM-S, MLB/SQFT-HR, TONS/SQFT-HR, L-TONS/SQFT-HR, TONNE/SQFT-HR
MASS-HEAT-CA	J/KG-K	BTU/LB-R	CAL/GM-K	KCAL/GM-K, PCU/LB-K, KJ/KG-K
MASS-OPER	KG/OP-SEC	LB/OP-HR	KG/OP-HR	LB/OP-SEC, MLB/OP-HR, TONS/OP-DAY, GM/OP-SEC, TONNE/OP-HR, LB/OP-DAY, KG/OP-DAY, TONS/OP-YEAR, TONS/OP-HR
MASS-PER-LEN	KG/M	LB/FT	KG/M	
MASS-TRANS-C	KG/S-SQM-KG/CUM	LB/HR-SQF-LB/CUF	GM/S-SQCM-GM/CC	
MASS-VOLUME	CUM/KG	CUFT/LB	CC/G	BPD/MLBPH, CC/KG
MOL-FLOW-LEN	KMOL/SEC-M	LBMOL/HR-FT	KMOL/HR-M	MOL/SEC-M, LBMOL/SEC-FT, LBMOL/DAY-FT, KMOL/DAY-M, MOL/MIN-M
MOLE-CONC	KMOL/CUM	LBMOL/CUFT	MOL/CC	MOL/L, MMOL/CC, MMOL/L
MOLE-CYCL	KMOL/CYCLE	LBMOL/CYCLE	KMOL/CYCLE	MMSCFH/CYCLE, MMSCMH/CYCLE, MOL/CYCLE, LBMOL/CYCLE, SCMH/CYCLE, LBMOL/CYCLE, KMOL/CYCLE, MMSCFD/CYCLE, SCFM/CYCLE
MOLE-DENSITY	KMOL/CUM	LBMOL/CUFT	MOL/CC	LBMOL/GAL, MOL/L
MOLE-ENTHALP	J/KMOL	BTU/LBMOL	CAL/MOL	KCAL/MOL, TCAL/MOL, MMKCAL/MOL, MMBTU/LBMOL, PCU/LBMOL, MMPCU/LBMOL, KJ/KMOL, GJ/KMOL, MJ/KMOL, KCAL/KMOL, GCAL/KMOL, MBTU/LBMOL, BTU/SCF, GCAL/MOL

Type of Units	SI Set	ENG Set	MET Set	Other Units Options
MOLE-ENTROPY	J/KMOL-K	BTU/LBMOL-R	CAL/MOL-K	KCAL/MOL-K, KJ/KMOL-K, TCAL/MOL-K, MJ/KMOL-K, KCAL/KMOL-K, GCAL/KMOL-K, MBTU/LBMOL-R
MOLE-FLOW	KMOL/SEC	LBMOL/HR	KMOL/HR	MMSCFH, MMSCMH, MOL/SEC, LBMOL/SEC, SCMH, LBMOL/DAY, KMOL/DAY, MMSCFD, MSCFD, SCFM, MOL/MIN, KMOL/KHR, KMOL/MHR, MOL/HR, MMOL/HR, MLBMOL/HR, LBMOL/MHR, LBMOL/MMHR, MSCFM, SCFH, MSCFH, SCFD, NCMH, NCMD
MOLE-HEAT-CA	J/KMOL-K	BTU/LBMOL-R	CAL/MOL-K	KCAL/MOL-K, TCAL/MOL-K, PCU/LBMOL-K, KJ/KMOL-K
MOLE-OPER	KMOL/OP-SEC	LBMOL/OP-HR	KMOL/OP-HR	MMSCF/CYCLE-HR, MMSCM/CYCLE-HR, MOL/OP-SEC, LBMOL/OP-SEC, SCM/CYCLE-HR, LBMOL/OP-DAY, KMOL/OP-DAY, MMSCF/CYCLE-DAY, SCF/CYCLE-MIN
MOLE-RXN-RATE	KMOL/CUM-S	LBMOL/CUFT-HR	KMOL/CUM-HR	MOL/CC-S
MOLE-VOLUME	CUM/KMOL	CUFT/LBMOL	CC/MOL	ML/MOL, BBL/MSCF
MOLES	KMOL	LBMOL	KMOL	SCM, MMSCF, MSCF, MMSCM, MOL, SCF
MOM-INERTIA	KG-SQM	LB-SQFT	KG-SQM	GM-SQCM, LB-SQIN
NUM-CON-RATE	NO/CUM-SEC	NO/CUFT-SEC	NO/L-SEC	NO/CC-SEC, NO/CUM-SEC, NO/CUM-MIN, NO/CUFT-MIN, NO/L-MIN, NO/CC-MIN, NO/CUM-HR, NO/CUFT-HR, NO/L-HR, NO/CC-HR
NUM-CONC	NO/CUM	NO/CUFT	NO/L	NO/CC, 1E6/CC
PACK-FACTOR	1/M	1/FT	1/M	
PDROP	N/SQM	PSI	ATM	LBF/SQFT, BAR, TORR, IN-WATER, KG/SQCM, MMHG, KPA, MM-WATER, MBAR, IN-WATER-60F, IN-HG, LB/FT-SQSEC, KG/M-SQSEC, PA, MPA, PSIA
PDROP-PER-HT	N/CUM	IN-WATER/FT	MM-WATER/M	MBAR/M, MMHG/FT
POP-DENSITY	NO/M/CUM	NO/FT/CUFT	NO/M/L	NO/MM/L, NO/MU/CC, NO/IN/CUIN
POWER	WATT	HP	KW	BTU/HR, CAL/SEC, FT-LBF/SEC, MW, GW, MJ/HR, KCAL/HR, GCAL/HR, MMBTU/HR, MBTU/HR, MHP
POWER-VOLUME	WATT/CUM	HP/CUFT	KW/L	KW/CUM
PRESSURE	N/SQM	PSI	ATM	LBF/SQFT, BAR, TORR, IN-WATER, KG/SQCM, MMHG, KPA, MM-WATER, MBAR, PSIG, ATMG, BARG, KG/SQCMG, LB/FT-SQSEC, KG/M-SQSEC, PA, MPA, PAG, KPAG, MPAG, MBARG, IN-HG, MMHG-VAC, IN-HG-VAC, IN-WATER-60F, IN-WATER-VAC, IN-WATER-60F-VAC, IN-WATER-G, IN-WATER-60F-G, MM-WATER-G, MM-WATER-60F-G, PSIA
RHO-VSQRD	KG/M-SQSEC	LB/FT-SQSEC	KG/M-SQSEC	
SIEMENS-M	SIEMENS/M	SIEMENS/FT	SIEMENS/M	SIEMENS/CM
SOLUPARAM	(J/CUM)**.5	(BTU/CUFT)**.5	(CAL/CC)**.5	(KCAL/CUM)**.5, (KJ/CUM)**.5, (CAL/ML)**0.5
SOLUTE-PERM	SQM/M-S	SQFT/FT-HR	SQM/M-HR	SQCM/CM-S, SQFT/FT-S
SOLVENT-PERM	KG/SQM-S-PA	LB/SQFT-HR-ATM	KG/SQM-HR-ATM	GM/SQCM-S-ATM, GM/SQCM-S-PA
SOUND-LEVEL	DECIBELS	DECIBELS	DECIBELS	
SPEC-FLT-RES	METER/KG	FT/LB	METER/KG	CM/GM
SPECIFICAREA	SQM/CUM	SQFT/CUFT	SQCM/CC	
SURFACE-TENS	N/M	DYNE/CM	DYNE/CM	LBF/FT, MN/M
TEMP-VOLUME	CUM-K/KMOL	CUFT-R/LBMOL	CC-K/MOL	

Type of Units	SI Set	ENG Set	MET Set	Other Units Options
TEMPERATURE	K	F	K	C, R
THERMAL-COND	WATT/M-K	BTU-FT/HR-SQFT-R	KCAL-M/HR-SQM-K	BTU-IN/HR-SQFT-R, C-CM/SEC-SQCM-K, CAL-CM/SEC-SQCM-K, BTU/HR-FT-R, KCAL/HR-M-K, J/SEC-M-K, KW/M-K
TIME	SEC	HR	HR	DAY, MIN, YEAR, MONTH, WEEK, NSEC
UA	J/SEC-K	BTU/HR-R	CAL/SEC-K	KJ/SEC-K, KCAL/SEC-K, KCAL/HR-K
UNIT-PRICE	$/KG	$/LB	$/KG	$/TON, $/MLB, $/GM, $/L-TON, $/TONNE, $/MMLB
VELOCITY	M/SEC	FT/SEC	M/SEC	MILE/HR, KM/HR, FT/MIN, MM/DAY, MM/HR, MM/DAY30, IN/DAY
VFLOW-LENGTH	SQM/SEC	GPM/FT	SQCM/SEC	SQM/HR, SQFT/MIN
VFLOW-RPM	CUM/SEC/RPM	CUFT/HR/RPM	L/MIN/RPM	GAL/MIN/RPM, GAL/HR/RPM, BBL/DAY/RPM, CUM/HR/RPM, CUFT/MIN/RPM, BBL/HR/RPM, CUFT/SEC/RPM, CUM/DAY/RPM, CUM/YEAR/RPM, L/HR/RPM, KBBL/DAY/RPM, MMCUFT/HR/RPM, MMCUFT/DAY/RPM, MCUFT/DAY/RPM, L/SEC/RPM, L/DAY/RPM, CUM/MIN/RPM
VISCOSITY	N-SEC/SQM	CP	CP	LB/FT-HR, MN-SEC/SQM, P, GM/SEC-CM, DYN-SEC/SQCM, PA-SEC
VOL-ENTHALPY	J/CUM	BTU/CUFT	CAL/CC	KCAL/CUM, KJ/CUM, MMBTU/BBL
VOL-HEAT-CAP	J/CUM-K	BTU/CUFT-R	CAL/CC-K	KCAL/CUM-K, KJ/CUM-K
VOLTAGE	VOLT	VOLT	VOLT	KVOLT
VOLUME	CUM	CUFT	L	CUIN, GAL, BBL, CC, KCUM, MCUM, MCUFT, MMCUFT, ML, KL, MML, MGAL, MMGAL, UKGAL, MUKGAL, MMUKGAL, MBBL, MMBBL, KBBL, CUYD
VOLUME-CYCL	CUM/CYCLE	CUFT/CYCLE	L/CYCLE	GAL/CYCLE, GAL/CYCLE, BBL/CYCLE, CUM/CYCLE, CUFT/CYCLE, BBL/CYCLE, CUFT/CYCLE, CUM/CYCLE, CUM/CYCLE, L/CYCLE, KBBL/CYCLE, MMCUFT/CYCLE
VOLUME-FLOW	CUM/SEC	CUFT/HR	L/MIN	GAL/MIN, GAL/HR, BBL/DAY, CUM/HR, CUFT/MIN, BBL/HR, CUFT/SEC, CUM/DAY, CUM/YEAR, L/HR, KBBL/DAY, MMCUFT/HR, MMCUFT/DAY, MCUFT/DAY, L/SEC, L/DAY, CUM/MIN, KCUM/SEC, KCUM/HR, KCUM/DAY, MCUM/SEC, MCUM/HR, MCUM/DAY, ACFM, CUFT/DAY, MCUFT/MIN, MCUFT/HR, MMCUFT/HR, MGAL/MIN, MMGAL/MIN, MGAL/HR, MMGAL/HR, MBBL/HR, MMBBL/HR, MBBL/DAY, MMBBL/DAY
VOLUME-OPER	CUM/OP-SEC	CUFT/OP-HR	L/OP-MIN	GAL/OP-MIN, GAL/OP-HR, BBL/OP-DAY, CUM/OP-HR, CUFT/OP-MIN, BBL/OP-HR, CUFT/OP-SEC, CUM/OP-DAY, CUM/OP-YEAR, L/OP-HR, KBBL/OP-DAY, MMCUFT/OP-HR
VOLUME-PRICE	$/CUM	$/CUFT	$/L	$/CC, $/BBL, $/CUYD, $/KL, $/CUIN, $/ML, $/MML, $/GAL, $/MGAL, $/MMGAL, $/UKGAL, $/MUKGAL, $/MMUKGAL, $/KBBL, $/MCUFT, $/MMCUFT, $/KCUM, $/MCUM, $/MBBL, $/MMBBL
VOLUME-USAGE	CUM/SEC	CUFT/HR	L/HR	L/DAY, L/YEAR, CUM/HR, CUM/DAY, CUM/YEAR
WATER-RATE	KG/J	LB/HP-HR	KG/KW-HR	
WORK	J	HP-HR	KW-HR	FT-LBF, KJ, N-M, MJ, MBTU, MMBTU, MCAL, GCAL

Label Definitions

The following table describes abbreviations used in Table 3.1:

Units	Description
MM	Used as a prefix meaning million before many units, such as MMBTU = million BTU.
M	Used as a prefix meaning thousand with English units, such as Mlb (thousand pounds) and Mscf (thousand standard cubic feet). With metric/SI units, the M prefix represents Mega except with millimeters and millinewtons.
SQ	Used as a prefix meaning squared, as in SQFT (square feet).
CU	Used as a prefix meaning cubed, as in CUM (cubic meters). The common abbreviation CC is used for cubic centimeters.
G	Used as a suffix on pressure units such as ATMG, BARG, PSIG, KG/SQCMG, and IN-WATER-G. The G indicates gauge pressure (pressure above standard atmospheric pressure).
VAC	Used as a suffix on pressure units such as IN-WATER-VAC, indicating vacuum pressure (pressure below standard atmospheric pressure). Vacuum units are thus exactly negative of the corresponding gauge pressure units.
IN-WATER, IN-WATER-60F	These units represent pressure in inches of water. IN-WATER is based on the density of water of 1 g/cc. IN-WATER-60F is based on the density of water at 60 F.
MMKCAL	Million kcal (same as GCAL)
MN	MilliNewtons
MLB	Thousand lbs
NCM	Normal cubic meters (same as standard cubic meters).
NCMH	Normal cubic meters per hour
NCMD	Normal cubic meters per day
PCU	Pound centrigrade unit
PSIA	Absolute pounds per square inch. PSI is a synonym for PSIA.
SCF	Standard cubic feet. Standard conditions for all standard cubic feet are ideal gas at 14.696 psi and 60 degrees F.
SCFH	Standard cubic feet per hour
SCFD	Standard cubic feet per day
SCM	Standard cubic meters. Standard conditions for all standard cubic meters are ideal gas at 1 atm and 0 degrees C.
SCMH	Standard cubic meters per hour
TONNE	Metric ton (1000 kg)

Rules for Entering Units

You must put single quotes (') around units with slashes (/), because the slash is a special character in Aspen Plus.

Units specified for one units keyword have no effect on other units keywords. For example, TIME may be in seconds, while MOLE-FLOW is in moles per hour.

You cannot enter units options using brackets or braces in the following cases:

- Vector input.
- Inline FORTRAN statements or expressions.
- PROP-DATA (see Chapter 8), DESIGN-SPEC (see Chapter 30), SENSITIVITY (see Chapter 35), CASE-STUDY (see Chapter 36), REPORT-SCALE (see Chapter 46), PROP-TABLE (see Chapter 40) or PROP-SET (see Chapter 41) paragraphs.
- HCURVE sentences of BLOCK paragraphs (see Chapter 11).
- SPEC and VARY sentences of RADFRAC, MULTIFRAC, PETROFRAC (see Chapter 15).

You must enter the pre-exponential factor and temperature exponent of the power law kinetics model in SI units, regardless of the IN-UNITS specification (see Chapters 6 and 19).

Custom Units of Measure

Use the **CUSTOM-UOM** paragraph to define custom units of measurement. You can define additional units for any of the physical quantity types in Aspen Plus.

For each unit you define, specify:

- The physical quantity type.
- A name for the unit.
- The base units, another unit of measurement of the same type. The new unit is defined with respect to this unit.
- A multiplier value.
- An offset value.

The multiplier and offset are the quantities needed to make this equation true:

1 custom unit = *multiplier* * base units + *offset*

For instance, if you wanted to define a foot in terms of inches, you would specify the base unit *inch*, multiplier 12, and offset 0.

Input Language for CUSTOM-UOM

CUSTOM-UOM
DEFINE-UOM *keyword=value*

Keywords:

PHYS-QTY **CUSTOM-UNIT** **BASE-UNIT** **MULTIPLIER**
OFFSET

Input Language Description for CUSTOM-UOM

DEFINE-UOM ..... Enter a DEFINE-UOM sentence for each custom unit of measurement.

PHYS-QTY ..... Physical quantity for custom units, such as LENGTH or TEMPERATURE. (Any of the **Units types** from table 3.1.)

CUSTOM-UNIT ..... Custom units. Alphanumeric string up to 20 characters

BASE-UNIT ..... Base units for the selected Physical Quantity, such as INCH or F.

MULTIPLIER ..... Multiplier in the equation: Quantity in Custom Units = Quantity in Base Units * Multiplier + Offset

OFFSET ..... Use sparingly! Offset in the equation: Quantity in Custom Units = Quantity in Base Units * Multiplier + Offset

4 Components

This chapter describes the input language for specifying components in a simulation. The paragraphs are:

Use this paragraph	To specify
COMPONENTS	Conventional components
FORMULA	Chemical formula for non-databank components
NC-COMPS	Component attributes for nonconventional components
HYPO-LIQ	Hypothetical liquid components
ATTR-COMPS	Component attributes for conventional components
COMP-GROUP	Component groups for plot and tear stream specification

Conventional Components

Input Language for COMPONENTS

```
COMPONENTS    cid    [cname]    [outid] / . . .
```

Input Language Description for COMPONENTS

Use the COMPONENTS paragraph to identify all components to include in a simulation. At least one component must be present in a simulation.

cid..... Component ID. You cannot use THRU as a component ID.

cname..... Name or alias used for the component in a databank. (See *APrSystem Physical Property Data*, Chapter 1.) Do not enter *cname* if component data are not to be retrieved from a databank, or if the component is not in a databank. When entering non-databank components, you may also want to use FORMULA (below) and STRUCTURES and PROP-DATA (see chapter 8).

outid..... Eight-character name used for the component in reports. If you want to enter *outid* but not *cname* for a component, place an asterisk (*) in the *cname* position. (Default=*cid*)

Input Language for FORMULA

```
FORMULA    cid    formula / . . .
```

Input Language Description for FORMULA

Use the FORMULA paragraph to specify chemical formulas for non-databank components. These formulas are only used for display purposes or as identifiers for components. To specify molecular formula, enter data for ATOMNO and NOATOM in a PROP-DATA paragraph (see chapter 8). To enter structural formulas, use a STRUCTURES paragraph (see chapter 8).

cid..... Component ID. You cannot use THRU as a component ID.

formula..... Chemical formula for non-databank component.

Nonconventional Components

Input Language for NC-COMPS

```
NC-COMPS    cid    cattrname-list
```

Input Language Description for NC-COMPS

Use the NC-COMPS paragraph to specify component attributes for nonconventional components.

cid..... Component ID. You cannot use THRU as a component ID.

cattrname-list..... List of component attributes for a nonconventional component. (See Table 4.1.)

Table 4.1 Component Attributes

Use this attribute	To
GENANAL	Define general constituent analysis for a compound. Its elements are analyzed in weight percent.
PROXANAL	Define the proximate analysis for coal. Its elements are analyzed in weight percent.
ULTANAL	Define the ultimate analysis for a compound on a dry basis. Its elements are analyzed in weight percent.
SULFANAL	Define the forms of sulfur analysis for coal on a dry basis. Its elements are analyzed in weight percent.
CAUSR1, CAUSR2, CAUSR3, CAUSR4, CAUSR5	Enter user-supplied component attribute information, for use in user models. The elements of this attribute type can correspond to whatever quantities you want.
BIOCOMP	Define the composition of a biomaterial. Its elements are analyzed in weight percent.
BIOSTATE	Define fraction of cell mass that is viable or dead
MACROSTATE	Describe the state of the component, such as protein

Hypothetical Liquid Component

Input Language for HYPO-LIQ

```
HYPO-LIQ    cid-list
```

Input Language Description for HYPO-LIQ

Use the HYPO-LIQ paragraph to specify solid components to use as reference state materials in a liquid solution. Aspen Plus generates liquid data sets for these components, based on solid data sets.

cid-list ..... List of component IDs

Component Attributes

Input Language for ATTR-COMPS

```
ATTR-COMPS    cid    cattrname-list
```

Input Language Description for ATTR-COMPS

Use the ATTR-COMPS paragraph to identify conventional components that you want to assign associated component attributes. In most cases, the conventional components you assign attributes to will be solids. You can assign attributes to non-solid conventional components, but Aspen Plus will not use these attributes in calculations.

cid ..... Component ID. You cannot use THRU as a component ID.

cattrname-list ..... List of component attributes for a conventional component. (See Table 4.1.)

Component Groups

Input Language for COMP-GROUP

```
COMP-GROUP    groupid    SUBSTREAM=ssid    COMPS=cid-list
```

Input Language Description for COMP-GROUP

Use the COMP-GROUP paragraph to specify component groups. A component group definition can consist of a list of components, a range of components from the COMPONENTS paragraph, or a combination of component lists and ranges. A component can appear in more than one group.

groupid ..... Component group ID. The group ID must not be the same as a component ID.

ssid ..... Substream ID

cid-list ..... List of component IDs or component ranges, cid_1 THRU cid_2

5 Chemistry and Electrolytes

This chapter describes the input language used to:

- Specify solution chemistry for electrolyte applications.
- Enter ternary parameters for the Pitzer property model.
- Access variables in CHEMISTRY.

Solution Chemistry

Input Language for CHEMISTRY

```
CHEMISTRY    chemid
DESCRIPTION  "a chemistry description - up to 64 characters in quotes"
PARAM        keyword=value
```

Optional keywords:

KBASIS TAPP

```
CALC-OPTIONS    keyword=value
```

Keywords:

HYDRATE-CHECK

```
DISS    electrolyteid    cid    coef  /  cid    coef  /  . . .
STOIC   reacno   cid    coef  /  cid    coef  /  . . .
K-STOIC   reacno   a    b    c    d
SALT    saltid   cid    coef  /  cid    coef  /  . . .
K-SALT    saltid   a    b    c    d
```

Input Language Description for CHEMISTRY

Solution chemistry can include the complete dissociation of strong electrolytes, partial dissociation of weak electrolytes, ionic reactions between or among ionic or molecular species, and precipitation of salts. Optionally, you can enter chemical equilibrium constants.

chemid ..... Chemistry ID

DESCRIPTION A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the CHEMISTRY paragraph report.

PARAM Use to specify the concentration scale of chemical-equilibrium constants and temperature approach for all reactions. The equilibrium constants are entered using the K-STOIC and K-SALT sentences.

KBASIS	**KBASIS=MOLEFRAC**	Mole fraction scale (Default)
	KBASIS=MOLAL	Molality scale
TAPP	Number of degrees of temperature approach to equilibrium. Aspen Plus calculates the chemical equilibrium constants at the system temperature plus TAPP. (Default=0)	

CALC-OPTIONS Use to specify calculation options.

HYDRATE-CHECK.....	**HYDRATE-CHECK= RIGOROUS**	Use a rigorous method to determine which hydrate to precipitate if multiple hydrates, including the anhydrous form, have been specified as salt precipitation reactions for any salt. Aspen Plus uses Gibbs free energy minimization when selecting the hydrate.
	HYDRATE-CHECK= APPROXIMATE	Use an approximate method to determine the hydrate. The hydrate selection is based on the lowest solubility product value at the system temperature.

DISS

Use to enter the complete dissociation reaction stoichiometry for strong electrolytes that dissociate completely. Salt dissociation/precipitation equilibrium is not considered for these electrolytes.

electrolyteid ..... Component ID of dissociating strong electrolytes

cid..... Component ID of a product of strong electrolytes dissociation

coef..... Stoichiometric coefficient (positive for products; negative for reactants other than dissociating strong electrolytes)

STOIC

Use to enter chemical-equilibrium ionic reaction stoichiometry.

reacno ..... Reaction number

cid..... Component ID

coef..... Stoichiometric coefficient (positive for products; negative for reactants)

K-STOIC

Use to enter the coefficients for the liquid-phase chemical-equilibrium constant expression for equilibrium reactions. If you do not use K-STOIC, Aspen Plus calculates chemical-equilibrium constants from the reference state free energies of the participating components. You must enter K-STOIC and STOIC sentences in the same order.

reacno ..... Reaction number used to identify the STOIC reaction

a,b,c,d..... Coefficients for equilibrium constant expression, which is defined as

$\ln(K) = a + b/T + c*\ln(T) + d*T$

Where:
K = Equilibrium constant
T = Temperature in Kelvin

SALT

Use to enter reaction stoichiometry for salt dissolution/precipitation, for salts that precipitate out of liquid solution.

saltid ..... Component ID of the precipitating salt

cid..... Component ID of a product of salt dissolution

coef..... Stoichiometric coefficient (positive for products; negative for reactants other than the dissoluting salt)

K-SALT

Use to enter the coefficients for the salt dissolution, chemical-equilibrium constant (solubility product) expression for equilibrium reactions. If you do not use K-SALT, Aspen Plus calculates chemical-equilibrium constants from the reference state free energies of the participating components.

saltid ..... Salt ID used to identify the SALT reaction

a,b,c,d..... Coefficients for equilibrium constant expression, which is defined as:

$\ln(K) = a + b/T + c*\ln(T) + d*T$

Where:
K = Equilibrium constant
T = Temperature in Kelvin

Pitzer Ternary Parameters

The Pitzer model requires ternary parameter Ψ. (See *APrSystem Physical Property Methods and Models*, Chapter 3 and Appendix C.) To enter parameter values for the ternary parameter Ψ (GMPTPS), use the standard PROP-DATA paragraph and BPVAL sentences with multiple elements (see Chapter 8). BPVAL provides entries for two component IDs. The element number provides another entry for the third component. You can determine the element number to use for a component from the component order in the COMPONENTS paragraph.

For example, enter $\Psi_{cac'}$ = .595 and $\Psi_{caa'}$ = .3049, for the following components:

```
COMPONENTS      H2O    H2O / c c / a a / c' c' / a' a'
```

Because component *c'* is the fourth component in the COMPONENTS paragraph, the value for $\Psi_{cac'}$ is entered as the fourth element in the BPVAL sentence. Component *a'* is the fifth component in the COMPONENTS paragraph, therefore the value for $\Psi_{caa'}$ is entered as the fifth element in the BPVAL sentence. An asterisk (*) is used as a place holder for the first, second, and third elements.

```
PROP-DATA
PROP-LIST   GMPTPS
BPVAL       c a   *  *  * .595   .3049
```

Accessing Variables in CHEMISTRY

Many Aspen Plus features enable you to sample or change chemistry variables. Chapter 29 describes how to access variables. The following table lists variable names and other information needed to sample and/or change variables.

Block Input

Sentence	Variables	ID1	ID2
PARAM	TAPP	—	—
STOIC	COEF	reacno	cid
K-STOIC	A, B, C, D	reacno	—
SALT	COEF	saltid	cid
K-SALT	A, B, C, D	saltid	—
DISS	COEF	electrolyteid	cid

6 Reactions

This chapter describes the input language for defining reactions and entering reaction data for use in distillation models, reactor models, and pressure relief systems. Reaction data include:

- Reaction stoichiometry.
- Reaction type.
- Parameters for kinetic and equilibrium constant expressions.

Four reactions paragraph types are available for defining reactions. The reaction paragraph types are:

Type	Purpose	Use
REAC-DIST	Define reactions for distillation models. Reactions can be equilibrium, rate-controlled, or fixed conversion type.	Referenced by distillation model RADFRAC
POWERLAW	Define power-law and equilibrium reactions for reactor models and pressure relief systems	Referenced by reactor models RCSTR, RPLUG, RBATCH, and PRES-RELIEF paragraph
LHHW	Define Langmuir-Hinshelwood-Hougen-Watson reactions for reactor models and pressure relief systems	Referenced by reactor models RCSTR, RPLUG, RBATCH, and PRES-RELIEF paragraph
USER	Define user kinetic and equilibrium reactions for reactor models, distillation models, and pressure relief systems	Referenced by reactor models RCSTR, RPLUG, and RBATCH; distillation model RADFRAC; and PRES-RELIEF paragraph

Defining Reactions for Distillation Models

Input Language for REAC-DIST

```
REACTIONS    reacid    REAC-DIST
DESCRIPTION  "a reaction description - up to 64 characters long"
REAC-DATA    reacno    [reactype]    keyword=value
```

Optional keywords:

PHASE DELT KBASIS CBASIS CONV-TYPE

```
STOIC    reacno    cid    coef  / cid    coef  / . . .
K-STOIC  reacno    a    b    c    d
RATE-CON  reacno    pre-exp    act-energy    [temp-exponent]    [t-ref]
POWLAW-EXP  reacno    cid    exponent
CONV  reacno    key-cid    conva    convb    convc    convd
SALT-DATA    salt-cid    keyword=value  / . . .
```

Optional keywords:

DELT KBASIS

```
SALT  salt-cid    cid    coef  / . . .
K-SALT    salt-cid    consta    constb    constc    constd  / . . .
PARAM    keyword=value
INT    value-list
REAL    value-list
```

Keywords:

SUBROUTINE NINT NREAL

Input Language Description for REAC-DIST

Use REAC-DIST to specify reactions to be considered within the RADFRAC model. Use the reaction ID to associate these reactions with segments of a distillation model. Equilibrium, rate-controlled, conversion, and salt dissociation reactions are allowed.

reacid..... Reaction ID

DESCRIPTION A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the REACTIONS paragraph report.

REAC-DATA Use to indicate the type of reaction and the phase in which the reaction occurs. You can also define the basis for the built-in equilibrium constant expression, the concentration basis for the built-in power-law kinetic expression, or the basis for the built-in fractional conversion expression.

reacno..... Reaction number

reactype..... Reaction type:

EQUIL	Equilibrium reaction (Default)
KINETIC	Rate-controlled reaction
CONV	Fractional conversion

PHASE ..... Phase where reaction occurs:

PHASE=L	Liquid (Default)
PHASE=L1	Liquid1
PHASE=L2	Liquid2
PHASE=V	Vapor

DELT ..... Number of degrees of temperature approach to equilibrium. Use for equilibrium reactions only. The equilibrium constant for the reaction is computed at the stage temperature + DELT. (Default=0)

KBASIS ..... Basis of equilibrium constant expression. All properties are for the phase specified in the REAC-DATA sentence. KBASIS is used only if K-STOIC is entered and *reactype* is EQUIL.

KBASIS=MOLE-GAMMA	$K = \pi(x_i \gamma_i)^{\upsilon_i}$ (Liquid phase only) (Default)
KBASIS=MOLAL-GAMMA	$K = \pi(C_i^m \gamma_i)^{\upsilon_i}$ (Electrolytes liquid phase only)
KBASIS=MOLEFRAC	$K = \pi(x_i)^{\upsilon_i}$
KBASIS=MASSFRAC	$K = \pi(x_i^m)^{\upsilon_i}$
KBASIS=MOLARITY	$K = \pi(C_i)^{\upsilon_i}$
KBASIS=MOLALITY	$K = \pi(C_i^m)^{\upsilon_i}$ (Electrolytes liquid phase only)
KBASIS=FUGACITY	$K = \pi(f_i)^{\upsilon_i}$
KBASIS=PARTIALPRES	$K = \pi(P_i)^{\upsilon_i}$ (Vapor phase only)
KBASIS=MASSCONC	$K = \pi(C_{m,i})^{\upsilon_i}$

Where:

K	=	Equilibrium constant
x	=	Component mole fraction
x^m	=	Component mass fraction
C	=	Molarity, (kgmole/m^3)
C^m	=	Molality (kgmole/kg-H_2O)
C_m	=	Mass concentration (kg/m^3)
γ	=	Activity coefficient
f	=	Component fugacity (N/m^2)
P	=	Partial pressure (N/m^2)
υ	=	Stoichiometric coefficient
i	=	Component index
π	=	Product operator

CBASIS ..... Concentration basis for power-law expression. Use for rate-controlled reactions only. CBASIS is used only if the power-law model is used and *reactype* is KINETIC or CONV.

CBASIS = MOLEFRAC $r = k(T/T_o)^n e^{-(E/R)[1/T-1/T_o]} \pi(x_i)^{\alpha_i}$

CBASIS = MASSFRAC $r = k(T/T_o)^n e^{-(E/R)[1/T-1/T_o]} \pi(x_i^m)^{\alpha_i}$

CBASIS = MOLARITY $r = k(T/T_o)^n e^{-(E/R)[1/T-1/T_o]} \pi(C_i)^{\alpha_i}$
(Default)

CBASIS = MOLALITY $r = k(T/T_o)^n e^{-(E/R)[1/T-1/T_o]} \pi(C_i^m)^{\alpha_i}$
(Electrolytes liquid phase only)

CBASIS=MASSCONC $r = k(T/T_o)^n e^{-(E/R)[1/T-1/T_o]} \pi(C_{m,i})^{\alpha_i}$

CBASIS=PARTIALPRES $r = k(T/T_o)^n e^{-(E/R)[1/T-1/T_o]} \pi(P_i)^{\alpha_i}$

Where:

r	=	Reaction rate
k	=	Pre-exponential factor
T	=	Temperature in Kelvin
T_o	=	Reference temperature in Kelvin
n	=	Temperature exponent
E	=	Activation energy
R	=	Universal gas law constant
x	=	Mole fraction
x^m	=	Mass fraction
C	=	Molarity (kgmole/m^3)
C^m	=	Molality (kgmole/kg-H_2O)
C_m	=	Mass concentration (kg/m^3)
P	=	Partial pressure (N/m^2)
α	=	Exponent
i	=	Component index
π	=	Product operator

CONV-TYPE ..... Fractional conversion type. You must specify *reactype* as CONV.

CONV-TYPE=SIMULT Simultaneous (Default)
CONV-TYPE=SERIES Series

STOIC Use to enter the stoichiometric coefficients for each reaction.

reacno..... Reaction number

cid..... Component ID

coef..... Stoichiometric coefficient (positive for products; negative for reactants)

K-STOIC Use to enter the coefficients for the equilibrium constant expression for equilibrium reactions. If you do not enter a K-STOIC sentence for a reaction, equilibrium constants are calculated from reference state free energies.

reacno..... Reaction number

a,b,c,d..... Coefficients for equilibrium constant expression, which is defined as:

$\ln(K) = a + b/T + c*\ln(T) + d*T$

Where:
K = Equilibrium constant
T = Temperature in Kelvin

RATE-CON

Use to enter parameters for the power-law expression for rate-controlled reactions. You must specify *reactype* as KINETIC.

reacno..... Reaction number

pre-exp..... Pre-exponential factor. Units must be in SI. (See the *Aspen Plus User Guide*.)

act-energy..... Activation energy. Units keyword is MOLE-ENTHALPY.

temp-exponent..... Temperature exponent for temperature in Kelvin (Default=0)

t-ref..... Reference temperature in Kelvin

POWLAW-EXP

Use to enter the component exponents for the power-law expression for rate-controlled reactions. If the order of the reaction with respect to a component is zero, you do not need to enter that component. You must also specify RATE-CON.

reacno..... Reaction number

cid..... Component ID

exponent..... Exponent. Does not need to be an integer.

CONV

Use to enter specifications for conversion-based reactions. You must specify the key component. You must also specify *reactype* as CONV in the REAC-DATA sentence. Specify either SERIES or SIMULTANEOUS for CONV-TYPE in the REAC-DATA sentence. When you specify multiple conversion reactions, they must have the same CONV-TYPE.

key-cid..... Key component ID

conva, convb, convc, convd..... Coefficients for fractional conversion expression, which is defined as:

CONV = (conva) + (convb)/T + (convc)*ln T + (convd)*T

Where:
CONV = Fractional conversion of key component
T = Temperature in Kelvin

SALT-DATA

Use to enter basis of user-defined equilibrium constants. You can also specify the temperature approach to equilibrium.

salt-cid..... Component ID of precipitating salt

DELT..... Number of degrees of temperature approach to equilibrium. The equilibrium constant for the reaction is computed at the stage temperature + DELT. (Default=0)

KBASIS..... Basis of user-defined equilibrium constants. You must also specify K-SALT.

KBASIS=MOLE-GAMMA $K = \pi(x_i \gamma_i)^{\upsilon_i}$ (Default)

KBASIS=MOLAL-GAMMA $K = \pi(C_i^m \gamma_i)^{\upsilon_i}$

KBASIS=MOLEFRAC $K = \pi(x_i)^{\upsilon_i}$

KBASIS=MASSFRAC $K = \pi(x_i^m)^{\upsilon_i}$

KBASIS=MOLARITY $K = \pi(C_i)^{\upsilon_i}$

KBASIS=MOLALITY $K = \pi(C_i^m)^{\upsilon_i}$

Where:

K	=	Equilibrium constant
x	=	Component mole fraction
x^m	=	Component mass fraction
C	=	Molarity (kgmole/m^3)
C^m	=	Molality (kgmole/kg-H_2O)
γ	=	Activity coefficient
υ	=	Stoichiometric coefficient
i	=	Component index
π	=	Product operator

SALT Use to define the stoichiometry for the salt precipitation/dissociation reactions.

salt-cid..... Component ID of precipitating salt

cid..... Component ID of components participating in the salt precipitation reaction

coef..... Stoichiometric coefficient

K-SALT Use to enter the coefficients for the salt dissociation equilibrium constant expression. If you do not enter the K-SALT sentence for a reaction, equilibrium constants are calculated from the reference state free energies.

salt-cid..... Component ID of precipitating salt

consta, constb..... constc, constd Coefficients for salt dissolution equilibrium constant expression, which is defined as:

ln(K) = consta + constb/T + constc*ln(T) + constd*T

Where:
K = Equilibrium constant
T = Temperature in Kelvin

PARAM Use to enter user-supplied kinetics subroutine name for reactive distillation calculations. For details on writing user-supplied kinetics subroutine, see *Aspen Plus User Models*, Chapter 11.

SUBROUTINE ..... User-supplied FORTRAN kinetics subroutine name

NINT ..... Length of integer parameter array

NREAL..... Length of real parameter array

INT Use to enter values for the integer parameter array of the user-supplied kinetics subroutine.

value-list..... List of integer values

REAL Use to enter values for the real parameter array of the user-supplied kinetics subroutine.

value-list..... List of real values

Defining Power-Law and Equilibrium Reactions for Reactors and Pressure Relief Systems

Input Language for POWERLAW

```
REACTIONS    reacid    POWERLAW
DESCRIPTION  "a reaction description - up to 64 characters long"
REAC-DATA    reacno    [reactype]    keyword=value
```

Optional keywords:

PHASE DELT KBASIS CBASIS SBASIS PH-BASIS-L PH-BASIS-S

```
STOIC    reacno  ssid  cid  coef /  cid  coef / . . .
K-STOIC  reacno  a  b  c  d
RATE-CON  reacno  pre-exp  act-energy  [temp-exponent]  [t-ref]
POWLAW-EXP  reacno  ssid  cid  exponent
```

Input Language Description for POWERLAW

Use POWERLAW to specify reactions parameters to be used with RCSTR, RPLUG, RBATCH, and PRES-RELIEF systems. Reactions can be equilibrium or rate-controlled, and can occur in the liquid or vapor phase.

reacid ..... Reaction ID

DESCRIPTION

A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the REACTIONS paragraph report.

REAC-DATA

Use to indicate the type of reaction and the phase in which the reaction occurs. You can also define the basis for the built-in equilibrium constant expression or the concentration basis for the built-in power-law kinetic expression. If solids are present in the system, use the SBASIS, PH-BASIS-L, and PH-BASIS-S keywords to provide information on how component concentrations are to be calculated.

reacno ..... Reaction number

reactype ..... Reaction type:

EQUIL	Equilibrium reaction
KINETIC	Rate-controlled reaction (Default)

PHASE..... Phase in which reaction occurs:

PHASE=L	Liquid (Default)
PHASE=L1	Liquid1
PHASE=L2	Liquid2
PHASE=LS	Liquid and solid
PHASE=V	Vapor

DELT ..... Number of degrees of temperature approach to equilibrium. Use for equilibrium reactions only. The equilibrium constant for the reaction is computed at the reactor temperature + DELT. DELT is allowed only when *reactype* is EQUIL. (Default=0)

KBASIS ..... Basis of equilibrium constant expression. All properties are for the phase specified in the REAC-DATA sentence. KBASIS is used only if K-STOIC is entered, and *reactype* is EQUIL.

KBASIS=MOLE-GAMMA $K = \pi(x_i \gamma_i)^{\upsilon_i}$ (Liquid phase only) (Default)

KBASIS=MOLAL-GAMMA $K = \pi(C_i^m \gamma_i)^{\upsilon_i}$ (Electrolytes liquid phase only)

KBASIS=MOLEFRAC $K = \pi(x_i)^{\upsilon_i}$

KBASIS=MASSFRAC $K = \pi(x_i^m)^{\upsilon_i}$

KBASIS=MOLARITY $K = \pi(C_i)^{\upsilon_i}$

KBASIS=MOLALITY $K = \pi(C_i^m)^{\upsilon_i}$ (Electrolytes liquid phase only)

KBASIS=FUGACITY $K = \pi(f_i)^{\upsilon_i}$

KBASIS=PARTIALPRES $K = \pi(P_i)^{\upsilon_i}$ (Vapor phase only)

KBASIS=MASSCONC $K = \pi(C_{m,i})^{\upsilon_i}$

Where:

K	=	Equilibrium constant
x	=	Component mole fraction
x^m	=	Component mass fraction
C	=	Molarity (kgmole/m^3)
C^m	=	Molality (kgmole/kg-H_2O)
C_m	=	Mass concentration (kg/m^3)
γ	=	Activity coefficient
f	=	Component fugacity (N/m^2)
P	=	Partial pressure (N/m^2)
υ	=	Stoichiometric coefficient
i	=	Component index
π	=	Product operator

CBASIS ..... Concentration basis for power-law expression. Use for rate-controlled reactions only. CBASIS is used only if *reactype* is KINETIC.

CBASIS = MOLEFRAC $r = k(T/T_o)^n e^{-(E/R)[1/T-1/T_o]}\pi(x_i)^{\alpha_i}$

CBASIS = MASSFRAC $r = k(T/T_o)^n e^{-(E/R)[1/T-1/T_o]}\pi(x_i^m)^{\alpha_i}$

CBASIS = MOLARITY $r = k(T/T_o)^n e^{-(E/R)[1/T-1/T_o]}\pi(C_i)^{\alpha_i}$
(Default)

CBASIS = MOLALITY $r = k(T/T_o)^n e^{-(E/R)[1/T-1/T_o]}\pi(C_i^m)^{\alpha_i}$
(Electrolytes liquid phase only)

CBASIS=MASSCONC $r = k(T/T_o)^n e^{-(E/R)[1/T-1/T_o]}\pi(C_{m,i})^{\alpha_i}$

CBASIS=PARTIALPRES $r = k(T/T_o)^n e^{-(E/R)[1/T-1/T_o]}\pi(P_i)^{\alpha_i}$
(Vapor phase only)

Where:

r	=	Reaction rate
k	=	Pre-exponential factor
T	=	Temperature in Kelvin
T_o	=	Reference temperature in Kelvin
n	=	Temperature exponent
E	=	Activation energy
R	=	Universal gas law constant
x	=	Mole fraction
x^m	=	Mass fraction
C	=	Molarity (kgmole/m^3)
C^m	=	Molality (kgmole/kg-H_2O)
C_m	=	Mass concentration (kg/m^3)
α	=	Exponent
P	=	Partial pressure (N/m^2)
i	=	Component index
π	=	Product operator

SBASIS ..... Basis for solid property calculations:

SBASIS=LOCAL	Solid property calculations are based on substream in which the component is present
SBASIS=GLOBAL	Solid property calculations are based on all solid substreams present (Default)

PH-BASIS-L ..... Liquid concentration basis:

PH-BASIS-L=L	Liquid phase calculations are based on liquid phase only (Default)
PH-BASIS-L=LS	Liquid phase calculations are based on liquid and solid phase

PH-BASIS-S ..... Solid concentration basis:

PH-BASIS-S=LS	Solid phase calculations are based on liquid and solid phase
PH-BASIS-S=S	Solid phase calculations are based on solid phase only (Default)

STOIC Use to enter the stoichiometric coefficients for each reaction.

reacno ..... Reaction number

ssid ..... Substream ID

cid ..... Component ID

coef ..... Stoichiometric coefficient (positive for products; negative for reactants)

K-STOIC Use to enter the coefficients for the equilibrium constant expression for equilibrium reactions. You must specify *reactype* as EQUIL. If you do not enter a K-STOIC sentence for a reaction, equilibrium constants are calculated from reference state free energies.

reacno ..... Reaction number

a,b,c,d ..... Coefficients for the equilibrium constant expression, which is defined as:

$\ln(K) = a + b/T + c*\ln(T) + d*T$

Where:
K = Equilibrium constant
T = Temperature in Kelvin

RATE-CON Use to enter parameters for the power-law expression for rate-controlled reactions. You must specify *reactype* as KINETIC.

reacno ..... Reaction number

pre-exp ..... Pre-exponential factor. Units must be in SI. (See the *Aspen Plus User Guide*.)

act-energy ..... Activation energy. Units keyword is MOLE-ENTHALPY.

temp-exponent ..... Temperature exponent for temperature in Kelvin (Default=0)

t-ref ..... Reference temperature in Kelvin

POWLAW-EXP Use to enter the component exponents for the power-law expression for rate-controlled reactions. If the order of the reaction with respect to a component is zero, that component need not be entered. You must also specify RATE-CON.

reacno ..... Reaction number

ssid ..... Substream ID

cid ..... Component ID

exponent ..... Exponent. Does not have to be an integer.

Defining LHHW Reactions for Reactors and Pressure Relief Systems

Input Language for LHHW

```
REACTIONS    reacid    LHHW
DESCRIPTIONS "a reaction description - up to 64 characters long"
PARAM        keyword=value
```

Keyword:

NTERM-ADS

```
REAC-DATA    reacno    [reactype]    keyword=value
```

Optional keywords:

PHASE DELT KBASIS CBASIS SBASIS PH-BASIS-L PH-BASIS-S

```
STOIC      reacno    ssid    cid    coef  /  cid    coef  /  . . .
K-STOIC    reacno    a    b    c    d
RATE-CON   reacno    pre-exp    act-energy    [temp-exponent]    [t-ref]
ADSORP-EXP   keyword=value  /  . . .
```

Keywords:

REACNO CID SSID EXPONENT

```
ADSORP-EQTER   reacno    term    a    b    c    d / . . .
ADSORP-POW     keyword=value  /  . . .
```

Keywords:

REACNO EXPONENT

```
DFORCE-EXP-1   reacno    ssid    cid    coef  /  ssid    cid    coef  /  . . .
DFORCE-EXP-2   reacno    ssid    cid    coef  /  ssid    cid    coef  /  . . .
DFORCE-EQ-1    reacno    a    b    c    d
DFORCE-EQ-2    reacno    a    b    c    d
```

Input Language Description for LHHW

Use LHHW to specify reaction parameters used with RCSTR, RPLUG, RBATCH, and PRES-RELIEF systems. Reactions can be equilibrium or rate-controlled, and can occur in the liquid or vapor phase. Kinetic reactions in this model follow the generalized Langmuir-Hinshelwood-Hougen-Watson model. By appropriate choice of the various model parameters, this model can be used to simulate other reaction rate forms such as Michaelis-Menten, Monod, or Powerlaw.

reacid ..... Reaction ID

DESCRIPTION A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the REACTIONS paragraph report.

PARAM Use to enter adsorption term parameters to specify optional kinetic data.

NTERM-ADS ..... Number of adsorption term parameters

REAC-DATA

Use to indicate the type of reaction and the phase in which the reaction occurs. You can also define the basis for the built-in equilibrium constant expression or the concentration basis for the built-in power-law kinetic expression. If solids are present in the system, use the SBASIS, PH-BASIS-L, and PH-BASIS-S keywords to provide information on how component concentrations are to be calculated.

reacno ..... Reaction number

reactype ..... Reaction type:

EQUIL	Equilibrium reaction
KINETIC	Rate-controlled reaction (Default)

PHASE..... Phase in which reaction occurs:

PHASE=L	Liquid (Default)
PHASE=L1	Liquid1
PHASE=L2	Liquid2
PHASE=LS	Liquid and solid
PHASE=V	Vapor

DELT ..... Number of degrees of temperature approach to equilibrium. Use for equilibrium reactions only. The equilibrium constant for the reaction is computed at the reactor temperature + DELT. DELT is allowed only when *reactype* is EQUIL. (Default=0)

KBASIS ..... Basis of equilibrium constant expression. All properties are for the phase specified in the REAC-DATA sentence. Use KBASIS only when K-STOIC is entered and *reactype* is EQUIL.

KBASIS=MOLE-GAMMA	$K = \pi(x_i \gamma_i)^{\upsilon_i}$ (Liquid phase only) (Default)
KBASIS=MOLAL-GAMMA	$K = \pi(C_i^m \gamma_i)^{\upsilon_i}$ (Electrolytes liquid phase only)
KBASIS=MOLEFRAC	$K = \pi(x_i)^{\upsilon_i}$
KBASIS=MASSFRAC	$K = \pi(x_i^m)^{\upsilon_i}$
KBASIS=MOLARITY	$K = \pi(C_i)^{\upsilon_i}$
KBASIS=MOLALITY	$K = \pi(C_i^m)^{\upsilon_i}$ (Electrolytes liquid phase only)
KBASIS=FUGACITY	$K = \pi(f_i)^{\upsilon_i}$
KBASIS=PARTIALPRES	$K = \pi(P_i)^{\upsilon_i}$ (Vapor phase only)
KBASIS=MASSCONC	$K = \pi(C_{m,i})^{\upsilon_i}$

Where:

K	=	Equilibrium constant
x	=	Component mole fraction
x^m	=	Component mass fraction
C	=	Molarity (kgmole/m^3)
C^m	=	Molality (kgmole/kg-H_2O)
C_m	=	Mass concentration (kg/m^3)
γ	=	Activity coefficient

f = Component fugacity (N/m^2)

P = Partial pressure (N/m^2)

υ = Stoichiometric coefficient

i = Component index

π = Product operator

CBASIS ..... Concentration basis for power-law expression. Use for rate-controlled reactions only. CBASIS is used only if *reactype* is KINETIC.

CBASIS = MOLEFRAC $r = k(T/T_o)^n e^{-(E/R)[1/T-1/T_o]} \pi(x_i)^{\alpha_i}$

CBASIS = MASSFRAC $r = k(T/T_o)^n e^{-(E/R)[1/T-1/T_o]} \pi(x_i^m)^{\alpha_i}$

CBASIS = MOLARITY $r = k(T/T_o)^n e^{-(E/R)[1/T-1/T_o]} \pi(C_i)^{\alpha_i}$
(Default)

CBASIS = MOLALITY $r = k(T/T_o)^n e^{-(E/R)[1/T-1/T_o]} \pi(C_i^m)^{\alpha_i}$
(Electrolytes liquid phase only)

CBASIS=MASSCONC $r = k(T/T_o)^n e^{-(E/R)[1/T-1/T_o]} \pi(C_{m,i})^{\alpha_i}$

CBASIS=PARTIALPRES $r = k(T/T_o)^n e^{-(E/R)[1/T-1/T_o]} \pi(P_i)^{\alpha_i}$
(Vapor phase only)

Where:

r = Reaction rate

k = Pre-exponential factor

T = Temperature in Kelvin

T_O = Reference temperature in Kelvin

n = Temperature exponent

E = Activation energy

R = Universal gas law constant

x = Mole fraction

x^m = Mass fraction

C = Molarity (kgmole/m^3)

C^m = Molality (kgmole/kg-H_2O)

C_m = Mass concentration (kg/m^3)

α = Exponent

P = Partial pressure (N/m^2)

i = Component index

π = Product operator

SBASIS ..... Basis for solid property calculations:

SBASIS=LOCAL	Solid property calculations are based on substream in which the component is present
SBASIS=GLOBAL	Solid property calculations are based on all solid substreams present (Default)

PH-BASIS-L..... Liquid concentration basis:

PH-BASIS-L=L	Liquid phase calculations are based on liquid phase only (Default)
PH-BASIS-L=LS	Liquid phase calculations are based on liquid and solid phase

PH-BASIS-S ..... Solid concentration basis:

PH-BASIS-S=S	Solid phase calculations are based on solid phase only (Default)
PH-BASIS-S=LS	Solid phase calculations are based on liquid and solid phase

STOIC

Use to enter the stoichiometric coefficients for each reaction.

reacno ..... Reaction number

ssid ..... Substream ID

cid..... Component ID

coef..... Stoichiometric coefficient (positive for products; negative for reactants)

K-STOIC

Use to enter the coefficients for the equilibrium constant expression for equilibrium reactions. You must specify *reactype* as EQUIL. If you do not enter a K-STOIC sentence for a reaction, equilibrium constants are calculated from reference state free energies.

reacno ..... Reaction number

a,b,c,d..... Coefficients for equilibrium constant expression, which is defined as:

$\ln(K) = a + b/T + c*\ln(T) + d*T$

Where:
K = Equilibrium constant
T = Temperature in Kelvin

RATE-CON

Use to enter parameters for the power-law expression for rate-controlled reactions. You must specify *reactype* as KINETIC.

reacno ..... Reaction number

pre-exp..... Pre-exponential factor. Units must be in SI. (See the *Aspen Plus User Guide*.)

act-energy ..... Activation energy. Units keyword is MOLE-ENTHALPY.

temp-exponent .. Temperature exponent for temperature in Kelvin (Default=0)

t-ref ..... Reference temperature in Kelvin

ADSORP-EXP

Use to enter exponents in adsorption expression terms. You must also specify ADSORP-EQTER and ADSORP-POW.

REACNO ..... Reaction number

CID ..... Component ID

SSID ..... Substream ID

EXPONENT ..... List of exponents for each concentration term in the adsorption expression. The number of values for EXPONENT must be equal to NTERM-ADS for at least one concentration term.

ADSORP-EQTER

Use to enter constant parameters in adsorption expression terms. You must also specify ADSORP-EXP and ADSORP-POW.

reacno ..... Reaction number

term..... Term number. The number of values for TERM must be equal to NTERM-ADS specified in the PARAM sentence.

a, b, c, d ..... Coefficients for adsorption expression, which is defined as:

$$\ln(K) = a + b/T + c*\ln(T) + d*T$$

Where:
K = Adsorption term constant
T = Temperature in Kelvin
Enter asterisk (*) for missing value.

ADSORP-POW

Use to enter adsorption term overall exponent. You must also specify ADSORP-EXP and ADSORP-EQTER.

REACNO ..... Reaction number

EXPONENT ..... Adsorption term overall exponent

DFORCE-EXP-1, DFORCE-EXP-2

Use to enter optional driving force exponents for reactants and products.

reacno ..... Reaction number

ssid..... Substream ID

cid..... Component ID

coef..... Exponent for the component in either the first or the second driving force expression. (See Note 1.)

DFORCE-EQ-1, DFORCE-EQ-2

Use to enter coefficients for calculating the driving force constants for the first and second driving force expressions defined in DFORCE-EXP-1 and DFORCE-EXP-2.

reacno ..... Reaction number

a, b, c, d ..... Parameters in the first and second driving force term. The expression is defined as:

$$\ln(K) = a + b/T + c*\ln(T) + d*T$$

Where:
K = Adsorption term constant
T = Temperature in Kelvin

Note

The general LHHW expression is: $r = \dfrac{(\text{kinetic factor})(\text{driving force expression})}{(\text{adsorption term})}$

kinetic factor = $k(T/T_o)^n e^{-(E/R)[1/T - 1/T_o]}$

driving force expression = $K_1\left(\prod_{i=1}^{N} C_i^{\alpha_i}\right) - K_2\left(\prod_{j=1}^{N} C_j^{\beta_j}\right)$

adsorption term = $\left[\sum_{i=1}^{M} K_i\left(\prod_{j=1}^{N} C_j^{\nu_j}\right)\right]^m$

Where:

r	=	Reaction rate
k	=	Pre-exponential factor
T	=	Absolute temperature
T_o	=	Reference temperature in Kelvin
n	=	Temperature exponent
m	=	Adsorption term exponent
E	=	Activation energy
R	=	Gas constant
K	=	Constant
K_1	=	Constant obtained from the driving force constants in DFORCE-EQ-1
K_2	=	Constant obtained from the driving force constants in DFORCE-EQ-2
N	=	Number of components
M	=	Number of terms in adsorption expression (NTERM-ADS)
i, j	=	Indices
α_i	=	Exponent for the component in the first term in the driving force expression
β_i	=	Exponent for the component in the second term in the driving force expression
ν	=	Term exponent for each component
Π	=	Product operator

Defining User-Kinetic and Equilibrium Reactions for Reactors, Distillation Models, and Pressure Relief Systems

Input Language for USER

```
REACTIONS    reacid    USER
DESCRIPTIONS   "a reaction description - up to 64 characters long"
REAC-DATA    reacno    [reactype]    keyword=value
```

Optional keywords:

PHASE DELT KBASIS SBASIS PH-BASIS-L PH-BASIS-S

```
STOIC    reacno    ssid    cid    coef  / cid    coef  / . . .
K-STOIC    reacno    a    b    c    d
PARAM    keyword=value
INT    value-list
REAL    value-list
```

Keywords:

SUBROUTINE NINT NREAL NIWORK NWORK

Input Language Description for USER

Use the USER model to specify reaction parameters to be used with reactor models RCSTR, RPLUG, and RBATCH; distillation model RADFRAC; and PRES-RELIEF systems. Reactions can be equilibrium or rate-controlled, and can occur in the liquid or vapor phase. The reaction rates in this model are calculated in a user-supplied subroutine.

reacid ..... Reaction ID

DESCRIPTION

A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the REACTIONS paragraph report.

REAC-DATA

Use to indicate the type of reaction and the phase in which the reaction occurs. You can also define the basis for the built-in equilibrium constant expression, or the concentration basis for the built-in power-law kinetic expression. If solids are present in the system, use the SBASIS, PH-BASIS-L, and PH-BASIS-S keywords to provide information on how component concentrations are to be calculated.

reacno ..... Reaction number

reactype ..... Reaction type:

EQUIL	Equilibrium reaction
KINETIC	Rate-controlled reaction (Default)

PHASE..... Phase in which reaction occurs:

PHASE=L	Liquid (Default)
PHASE=L1	Liquid1
PHASE=L2	Liquid2

PHASE=LS Liquid and solid

PHASE=V Vapor

DELT ..... Number of degrees of temperature approach to equilibrium. Use for equilibrium reactions only. The equilibrium constant for the reaction is computed at the reactor temperature + DELT. DELT is allowed only when *reactype* is EQUIL. (Default=0)

KBASIS ..... Basis of equilibrium constant expression. All properties are for the phase specified in the REAC-DATA sentence. KBASIS is used only if K-STOIC is entered and *reactype* is EQUIL.

KBASIS=MOLE-GAMMA $K = \pi(x_i \gamma_i)^{\upsilon_i}$ (Liquid phase only) (Default)

KBASIS=MOLAL-GAMMA $K = \pi(C_i^m \gamma_i)^{\upsilon_i}$ (Electrolytes liquid phase only)

KBASIS=MOLEFRAC $K = \pi(x_i)^{\upsilon_i}$

KBASIS=MASSFRAC $K = \pi(x_i^m)^{\upsilon_i}$

KBASIS=MOLARITY $K = \pi(C_i)^{\upsilon_i}$

KBASIS=MOLALITY $K = \pi(C_i^m)^{\upsilon_i}$ (Electrolytes liquid phase only)

KBASIS=FUGACITY $K = \pi(f_i)^{\upsilon_i}$

KBASIS=PARTIALPRES $K = \pi(P_i)^{\upsilon_i}$ (Vapor phase only)

KBASIS=MASSCONC $K = \pi(C_{m,i})^{\upsilon_i}$

Where:

K	=	Equilibrium constant
x	=	Component mole fraction
xm	=	Component mass fraction
C	=	Molarity (kgmole/m^3)
C^m	=	Molality (kgmole/kg-H_2O)
C_m	=	Mass concentration (kg/m^3)
γ	=	Activity coefficient
f	=	Component fugacity (N/m^2)
P	=	Partial pressure (N/m^2)
υ	=	Stoichiometric coefficient
i	=	Component index
π	=	Product operator

SBASIS ..... Basis for solid property calculations:

SBASIS=LOCAL Solid property calculations are based on substream in which the component is present

SBASIS=GLOBAL Solid property calculations are based on all solid substreams present (Default)

PH-BASIS-L..... Liquid concentration basis:

	PH-BASIS-L=L	Liquid phase calculations are based on liquid phase only (Default)
	PH-BASIS-L=LS	Liquid phase calculations are based on liquid and solid phase

PH-BASIS-S ..... Solid concentration basis:

PH-BASIS-S=S	Solid phase calculations are based on solid phase only (Default)
PH-BASIS-S=LS	Solid phase calculations are based on liquid and solid phase

STOIC

Use to enter the stoichiometric coefficients for each reaction.

reacno ..... Reaction number

ssid ..... Substream ID

cid ..... Component ID

coef ..... Stoichiometric coefficient (positive for products; negative for reactants)

K-STOIC

Use to enter the coefficients for equilibrium constant expression for equilibrium reactions. If a K-STOIC sentence is not entered for a reaction, equilibrium constants are calculated from reference state free energies.

reacno ..... Reaction number

a,b,c,d ..... Coefficients for equilibrium constant expression, which is defined as:

$\ln(K) = a + b/T + c*\ln(T) + d*T$

Where:
K = Equilibrium constant
T = Temperature in Kelvin

PARAM

Use to specify user-supplied kinetics subroutine. For details on writing user-supplied kinetics subroutine, see *Aspen Plus User Models*, Chapter 11.

SUBROUTINE ..... User-supplied FORTRAN kinetics subroutine name

ORIGIN ..... Type of argument list used by Aspen Plus in calling the user-supplied Fortran kinetics subroutine.

ORIGIN=SYSTEM	New argument list compatible for reactors, separation, and pressure relief blocks
ORIGIN=RBATCH	Old argument list compatible for RBATCH blocks only
ORIGIN=RPLUG	Old argument list compatible for RPLUG blocks only
ORIGIN=RCSTR	Old argument list compatible for RCSTR blocks only

The argument list for ORIGIN=SYSTEM is described in *Aspen Plus User Models*, Chapter 11. Do not use ORIGIN=RCSTR, RBATCH, or RPLUG for new simulations. They are available only to provide upward compatibility with pre-Version 10 simulations that specified the user kinetics subroutine as part of the block input specifications.

NINT ..... Length of integer parameter array

NREAL ..... Length of real parameter array

NIWORK ..... Length of integer workspace array

NWORK ..... Length of real workspace array

INT Use to enter values for the integer parameter array of the the user-supplied kinetics subroutine.

value-list ..... List of integer values

REAL Use to enter values for the real parameter array of the user-supplied kinetics subroutine.

value-list ..... List of real values

Accessing Variables in REACTIONS

Many Aspen Plus features enable you to sample or change reaction variables. Chapter 29 describes how to access variables. The following table lists variable names and other information needed to sample and/or change variables.

Block Input

Sentence	Variables	ID1	ID2	ID3	Element
REAC-DATA	DELT	reacno	—	—	—
STOIC	COEF	reacno	†	††	—
K-STOIC	a, b, c, d	reacno	—	—	—
CONV	conva, convb, convc, convd	reacno	—	—	—
RATE-CON	PRE-EXP, ACT-ENERGY, TEMP-EXPONENT	reacno	—	—	—
POWLAW-EXP	EXPONENT	reacno	†††	††	—
K-SALT	consta, constb constc, constd	saltid	—	—	—
DFORCE-EXP-1	DF1-EXP	reacno	ssid	cid	—
DFORCE-EXP-2	DF2-EXP	reacno	ssid	cid	—
DFORCE-EQ-1	DF1-A, DF1-B, DF1-C, DF1-D	reacno	—	—	—
DFORCE-EQ-2	DF2-A, DF2-B, DF2-C, DF2-D	reacno	—	—	—
ADSORP-EXP	ADS-EXPONENT	reacno	cid	ssid	♦
ADSORP-EQTER	ADS-A, ADS-B ADS-C, ADS-D	reacno	termno	—	—
ADSORP-POW	ADS-PW-EXP	reacno	—	—	—
INT	VALUE-LIST	—	—	—	♦
REAL	VALUE-LIST	—	—	—	♦

† Use cid for REAC-DIST; use ssid for POWERLAW, LHHW, and USER.

†† Use cid for POWERLAW, LHHW, and USER.

††† Use cid for REAC-DIST; use ssid for POWERLAW.

♦ Position of a value in the ADSORP-EXP, INT, or REAL value-list.

7 Petroleum Assays and Pseudocomponents

This chapter describes the input language for:

- Specifying assay analysis options.
- Entering assay data for petroleum streams.
- Defining a new petroleum property.
- Blending assays.
- Generating pseudocomponents from assays and blends.
- Defining individual pseudocomponents.
- Defining and modifying pseudocomponent property correlation option sets.
- Entering properties for pseudocomponents.

Specifying Assay Analysis Options

Input Language for ADA-SETUP

ADA-SETUP	*keyword=value*

Optional keywords:

PROCEDURE D86-METH D2887-METH D1160-METH MW-INTGR-H EXTRAP-METH IBP EP SPLINE-FIT

Input Language Description for ADA-SETUP

ADA-SETUP

Use to specify assay analysis options. You must enter PROCEDURE=REL9 to modify the options.

PROCEDURE ..... Assay analysis procedure:

PROCEDURE=REL9	Uses Release 9 procedures. These procedures provide a more accurate representation for distillation curves. You must use the REL9 procedure if you are entering D2887 distillation curve or PROP-CURVE sentences in the ASSAY paragraph. (Default)
PROCEDURE=PRE-REL9	Uses pre-Release 9 procedures

D86-METH ..... Procedure for converting D86 distillation curve to TBP basis:

D86-METH=EDMISTER	Uses the Edmister conversion procedure (Default)
D86-METH=ED-OK	Uses the Edmister-Okamato conversion procedure
D86-METH=API94	Uses the conversion procedure from the 1994 API Technical Data Book
D86-METH=API92	Uses the conversion procedure from the 1992 API Technical Data Book
D86-METH=PML	Uses the conversion procedure developed by AspenTech. It is similar to the API method, but uses its own conversion correlation.

D2887-METH ..... Procedure for converting D2887 distillation curve to TBP basis:

D2887-METH=API87	Uses the conversion procedure from the 1987 API Technical Data Book
D2887-METH=API94	Uses the conversion procedure from the 1994 API Technical Data Book (Default)
D2887-METH=TBPWT	The D2887 data entered are treated as True boiling point data based on weight percent

D1160-METH ..... Procedure for converting D1160 distillation curve to TBP basis:

D1160-METH=API63	Uses the conversion procedure from the 1963 API Technical Data Book (Default)
D1160-METH=PML	Uses the conversion procedure developed by AspenTech. It is similar to the API method, but uses its own conversion correlation.

MW-INTGR-H ..... Minimum step size for molecular weight curve integration. (Default=0.1)

EXTRAP-METH..... Distillation curve extrapolation method:

EXTRAP-METH= PROBABILITY	Extrapolates distillation curve using normal probability distribution function. (Default)
EXTRAP-METH= QUADRATIC	Extrapolates distillation curve using a quadratic fit of the last three points.

IBP ..... Initial boiling point. Use for distillation curve extrapolation. (Default=0.5)

EP ..... Final boiling point. Use for distillation curve extrapolation. (Default=99.0)

SPLINE-FIT ..... Method used for curve fitting

HARWELL	Use Harwell cubic splines (Default)
HERMITE	Use Hermite cubic splines
LINEAR	Use linear method

Entering Assay Data for Petroleum Streams

Input Language for ASSAY

```
ASSAY    assayid
ASSAY-DATA    keyword=value
```

Optional keywords:

GRAV API VACPRES LE-FRAC MW CRACK-OPT MATCH-LTENDS

```
DIST-CURVE    disttype    pct-dist    temp  /  pct-dist    temp  /  . . .
GRAV-CURVE    gravtype    mid-pct    grav  /  mid-pct    grav  /  . . .
UOPK-CURVE    mid-pct    uopk  /  mid-pct    uopk  /  . . .
MW-CURVE    mid-pct    mw  /  mid-pct    mw  /  . . .
LE-basis-FRAC    cid    frac    [grav]    [mw]  /  . . .
CONVERT    disttype-list
PROP-CURVE    propname    mid-pct    propvalue  /  mid-pct    propvalue  /  . . .
BULK-PROP    propname    propvalue
VISC-CURVE    temp    mid-pct    visc  /  . . .
KVISC-CURVE    temp    mid-pct    visc  /  . . .
```

Input Language Description for ASSAY

Use the ASSAY paragraph to enter assay data, including the amount of any light end component identified in the mixture. ASSAY-DATA and DIST-CURVE are required; all other sentences are optional.

assayid ..... Assay ID. This keyword cannot be the same as a component ID.

ASSAY-DATA

Use to enter optional parameters that apply to the entire assay. If you do not enter the GRAV-CURVE sentence. You must enter either GRAV or API. For the proper use of LE-FRAC and MW, see LE-basis-FRAC.

GRAV ..... Specific gravity

API ..... API gravity

VACPRES..... Distillation pressure. Use this keyword if *disttype* is D1160, VACLV, or VACWT. (Default=10 mm Hg)

LE-FRAC..... Light end fraction

MW ..... Molecular weight

CRACK-OPT..... Cracking correction code for D86 distillation data:

CRACK-OPT=YES	Standard API cracking correction is applied to the temperature that you enter using DIST-CURVE
CRACK-OPT=NO	No correction is applied (Default)

MATCH-LTENDS..... Specifies whether to adjust the distillation curve to match light-ends analysis data.

MATCH-LTENDS=YES	Adjusts distillation curve
MATCH-LTENDS=NO	Does not adjust distillation curve (Default)

DIST-CURVE

Use to enter distillation temperatures versus percent distilled. A minimum of four points in ascending order is required. If you do not enter a temperature for the 100 percent point, Aspen Plus extrapolates the data to 100 percent. If you do not want extrapolation, normalize the data. As pen Plus extrapolates or interpolates the data to a percentage equal to the amount of light end components specified.

disttype	**D86**	ASTM D86
	D1160	ASTM D1160
	TBPLV	True boiling point (liquid volume basis)
	TBPWT	True boiling point (weight basis)
	VACLV	Vacuum (liquid volume basis)
	VACWT	Vacuum (weight basis)
	D2887	ASTM D2887
pct-dist	Percent distilled	
temp	Temperature	

GRAV-CURVE

Use to enter gravity data. Gravities supplied in the GRAV-CURVE sentence are normalized to match the API or GRAV value given in the ASSAY-DATA sentence. A minimum of four points is required.

gravtype	**GRAV**	Specific gravity
	API	API gravity
mid-pct	Mid-percent distilled. Aspen Plus uses the same basis as that used for distillation data (for example, volume or weight).	
grav	Gravity	

UOPK-CURVE

Use to enter Watson UOP K data. If you enter GRAV-CURVE, you do not need to enter UOPK-CURVE. A minimum of four points is required. If *disttype* is TBPWT, VACWT, or D2887, you cannot enter UOPK-CURVE.

mid-pct	Mid-percent distilled on a volume basis. Aspen Plus uses the same basis as that used for distillation data (for example, volume or weight).
uopk	Watson UOP K

MW-CURVE

Use to enter molecular weight data. If you enter MW in the ASSAY-DATA sentence, Aspen Plus normalizes the values supplied in the MW-CURVE sentence. A minimum of four points is required.

mid-pct	Mid-percent distilled. Aspen Plus uses the same basis as that used for distillation data (for example, volume or weight).
mw	Molecular weight

LE-basis-FRAC

Use to enter a light end analysis on a MOLE, MASS, or STDVOL (standard-liquid- volume) basis.

cid	Component ID
frac	If you enter LE-FRAC in the ASSAY-DATA sentence, Aspen Plus normalizes the *frac* values. If you do not enter LE-FRAC, Aspen Plus treats the *frac* values as fractions of the entire assay mixture. You must enter the molecular weight (MW) of the assay in the ASSAY-DATA sentence if you use LE-MOLE-FRAC.
grav	Specific gravity (Default=databank value)
mw	Molecular weight (Default=databank value)

CONVERT Use to request conversion of the distillation data to other bases for report purpose only. Distillation curves on a TBP basis and the basis used for DIST-CURVE input are always reported.

disttype-list ..... One or more of the following: D86, D1160, VACLV

PROP-CURVE Use to enter any number of property curves for the assay. A variety of built-in curve types are allowed. You can also define a new property using the PETRO-PROP paragraph. Based on these curves, property values are assigned to individual pseudocomponents in the simulation.

propname ..... Property name from Table 7.1 or as defined in a PETRO-PROP paragraph

mid-pct ..... Mid-percent distilled on a standard-liquid-volume basis

propvalue ..... Property value

BULK-PROP Use to enter the bulk value for property curves. Aspen Plus uses this value to normalize individual curve values specified in the PROP-CURVE sentence.

propname ..... Property name from Table 7.1 or as defined in a PETRO-PROP paragraph

propvalue ..... Bulk value for property curve

VISC-CURVE Use to enter optional absolute viscosity curves as a function of percent distilled for an assay. You can enter the curves at different temperatures. Based on these curves, Aspen Plus assigns viscosity to the pseudocomponents generated for the assay. You cannot use VISC-CURVE if you specify KVISC-CURVE.

temp ..... Temperature for viscosity curve

mid-pct ..... Mid-percent distilled on a standard-liquid-volume basis

visc ..... Absolute viscosity value

KVISC-CURVE Use to enter optional kinematic viscosity curves as a function of percent distilled for an assay. You can enter the curves at different temperatures. Based on these curves, Aspen Plus assigns viscosity to the pseudocomponents generated for the assay. You cannot use KVISC-CURVE if you specify VISC-CURVE.

temp ..... Temperature for viscosity curve

mid-pct ..... Mid-percent distilled on a standard-liquid-volume basis

visc ..... Kinematic viscosity value

Table 7.1 Petroleum Properties

Property	Description	Default Blending Method
ANILPT	Aniline point	MASS
AROMATIC	Aromatic content	STDVOL
ASPHALTE	Asphaltene content	MASS
BASIC-N2	Basic nitrogen content	MASS
BROMINE	Bromine number	MASS
CARBON	Carbon residue	MASS
CETANE	Cetane number	MASS
CLOUDPT	Cloud point	MASS
COCARBON	Conradson carbon	MASS
FLASHPT	Flash point	MASS
FREEZEPT	Freeze point	MASS
HYDROGEN	Hydrogen content	STDVOL
IRON	Iron content	MASS
KNOCKIDX	Antiknock index	MASS
KVISC	Kinematic viscosity	MASS
LUMI-NO	Luminometer number	STDVOL
MERCAPTA	Mercaptan content	MASS
METAL	Metal content	STDVOL
MOC-NO	Motor octane number	STDVOL
NAPHTHEN	Naphthene content	MASS
NICKEL	Nickel content	MASS
OLEFIN	Olefin content	STDVOL
OXYGEN	Oxygen content	STDVOL
PARAFFIN	Paraffin content	MASS
POURPT	Pour point	MASS
REFINDEX	Refractive index	MASS
ROC-NO	Research octane number	STDVOL
RVP	Reid vapor pressure	MASS
SMOKEPT	Smoke point	MASS
SULFUR	Sulfur content	MASS
TOTAL-N2	Total nitrogen content	MASS
VANADIUM	Vanadium content	MASS
VISC	Viscosity	MASS
VLOCKIDX	Vapor lock index	MASS
WARMIDX	Warm-up index	MASS

Defining a New Petroleum Property

Input Language for PETRO-PROP

```
PETRO-PROP    propname    keyword=value
```

Keywords:

BLEND-METHOD BLEND-OPTION EXTRAPOLATE

Input Language Description for PETRO-PROP

Use the PETRO-PROP paragraph to define a new petroleum property, or to modify the calculation options of a built-in petroleum property. The calculation options are:

propname ..... Property name. Specify a new property name, or a built-in property from Table 7.1.

BLEND-METHOD..... Blending method. The available methods are MOLE, MASS, STDVOL, and USER. Table 7.1 describes the defaults.

BLEND-OPTION..... Option code for use in the user blending subroutine if BLEND-METHOD=USER is specified. The code is passed unchanged to the user-blending routine through the argument list.

EXTRAPOLATE..... Curve extrapolation code:

EXTRAPOLATE=YES	Extrapolates property curve, if it does not encompass the entire composition range (Default)
EXTRAPOLATE=NO	Does not extrapolate property curve

Blending Assays

Input Language for BLEND

```
BLEND    blendid
basis-FRAC    assayid    frac  /  ...
CONVERT    disttype-list
```

Input Language Description for BLEND

Use the BLEND paragraph to request that two or more assays blend to create a new assay. An assay generated by blending, can itself be blended.

blendid..... Blend ID. The blend ID cannot be the same as a component ID.

basis-FRAC Use to enter the fractions of each assay in the blend on a MOLE, MASS, or STDVOL basis.

assayid ..... Assay ID

Frac ..... Mole, mass, or standard-liquid-volume fraction

CONVERT Use to request conversion of the distillation data to other bases for report purposes only. Distillation curves on a TBP basis and the basis used for DIST-CURVE input are always reported.

disttype-list ..... One or more of the following: D86, D1160, VACLV

Generating Pseudocomponents from Assays and Blends

Input Language for PC-CALC

```
PC-CALC
PC-SET    assayid    [wf]  /  . . .
CUTS { LIST = value – list                                  } { NINC = ninc } / UTEMP = utemp { NINC = ninc } /...
     { LTEMP = ltemp UTEMP = utemp                          } { INCR = incr }                { INCR = incr }
PROPS     pcopsetname
NOPROPS   pcopsetname
PC-IDS    keyword=value
```

Optional keywords:

OPTION LIST FIRST-NO

Input Language Description for PC-CALC

Use the PC-CALC paragraph to generate a set of pseudocomponents from assay data. Use a separate PC-CALC paragraph for each set of components generated. All sentences of PC-CALC are optional. If you do not enter PC-CALC paragraphs, Aspen Plus generates an average set of pseudocomponents for all assays present.

PC-SET Use to enter a list of assays to include when generating a pseudocomponent set. If you do not enter PC-SET, all assays are included with equal weight.

assayid ..... Assay ID

wf ..... Weighting factors for each assay (Default=1)

CUTS Use to enter the temperature cut points to use in generating pseudocomponents. You can indicate the cuts as a list of values. Or you can indicate the cuts as the number of increments or size of increments within a given temperature range. If you do not enter CUTS, Aspen Plus uses the following default cut points:

TBP Range °F	Number of Cuts	Increments °F
100- 800	28	25
800-1200	8	50
1200-1600	4	100

LIST ..... List of cut points

LTEMP, UTEMP ..... Lower and upper temperatures of a range divided into increments. (When more than one range is provided, the lower temperature is assumed to equal the upper temperature of the previous range.)

NINC ..... Number of increments

INCR ..... Size of increments

PROPS

Use to specify the correlation option set for estimating pseudocomponent properties. Specify one of the five built-in correlation option sets (see Table 7.2) or a *pcopsetname* defined in a PC-PROP-OPT paragraph.

pcopsetname ..... PC correlation option set name (Default=ASPEN)

NOPROPS

Use to request that pseudocomponent properties not be calculated. Aspen Plus uses the molecular weight correlation when properties are not calculated. So you must use *pcopsetname* with NOPROPS. See PROPS for *pcopsetname* options.

PC-IDS

Use to specify component IDs for the system-generated pseudocomponents. The component ID is the number preceded by the characters PC except when OPTION=LIST.

OPTION..... Naming option:

OPTION=LIST	IDs specified by LIST keyword
OPTION=NBP	Average boiling point (Default)
OPTION=NUMBERED	Sequential numbers starting with the value specified by FIRST-NO
OPTION=ROUND-UP	Upper cut temperature
OPTION=ROUND-DOWN	Lower cut temperature

LIST..... List of component IDs, required when OPTION=LIST

FIRST-NO..... Number used in ID of first pseudocomponent. Use this number when OPTION=NUMBERED. (Default=1)

Table 7.2 Pseudocomponent Correlation Option Set

	PC Correlation Option Set				
Property	**API-METH Model**	**COAL-LIQ Model**	**ASPEN Model**	**LK Model**	**API-TWU Model**
Molecular weight	MWHS	MWHS	HS-ASPEN	MWKL	HS-ASP
Critical temperature	TCRZI	TCASPN	TCRZI	TCKL	TCTWU
Critical pressure	PCRZI	PCASPN	PCRZI	PCKL	PCTWU
Critical volume	VCRDL	VCRDL	VCRDL	VCRDL	VCTWU
Vapor pressure	PLMB	PLSWAP	BK-10	PLKL	BK-10
Ideal gas heat capacity	CPIGKL	CPMM	CPIGKL	CPIGKL	CPIGKL
Liquid molar volume	VLRKT	VLRKT	VLRKT	VLRKT	VLRKT
Enthalpy of vaporization	DHVLVET	DHVLVET	DHVLVET	DHVLVET	DHVLVET
Acentric factor	OMEGAKL	OMEGAKL	KL-ASPEN	OMEGAKL	KL-ASPEN
Viscosity	MULWAT	MULWAT	MULWAT	MULWAT	MULWAT
BWR orientation parameter	GMASTAR	GMASTAR	GMASTAR	GMASTAR	GMASTAR
BWR critical temperature	TCSTAR	TCSTAR	TCSTAR	TCSTAR	TCSTAR
BWR critical volume	VCSTAR	VCSTAR	VCSTAR	VCSTAR	VCSTAR
Standard enthalpy of formation	DHFMZERO	DHFMZERO	DHFMONT	DHFMONT	DHFMONT
Standard free energy of formation	DGFMZERO	DGFMZERO	DGFMONT	DGFMONT	DGFMONT
RKS interaction parameters	API78	API78	API78	API78	API78
Water solubility	WSOLASPN	WSOLASPN	WSOLASPN	WSOLASPN	KEROSENE

Defining Individual Pseudocomponents

Input Language for PC-USER

```
PC-USER
PC-DEF    pcopsetname    pcid    keyword=value
```

Keywords:

NBP API GRAV LDEN MW

Input Language Description for PC-USER

Use the PC-USER paragraph to enter user-defined pseudocomponents. Enter one PC-DEF sentence for each user-defined pseudocomponent. You must enter user-defined pseudocomponent IDs as component IDs in the COMPONENTS paragraph.

PC-DEF

Use to enter user-defined pseudocomponents. You must supply at least two of the following properties: normal boiling point, gravity (or density), and molecular weight. To enter additional property data for user-defined pseudocomponents, use the PC-PROP-DATA paragraph (this chapter) or the PROP-DATA paragraph (see Chapter 8). Required property parameters not entered in these paragraphs are estimated.

pcopsetname	PC correlation option set name. Specify one of the five built-in option sets (see Table 7.2) or a new PC option set defined using the PC-PROP-OPT paragraph. (Default=ASPEN)
pcid	Pseudocomponent ID
NBP	Normal boiling point
API	API gravity
GRAV	Specific gravity
LDEN	Standard liquid density
MW	Molecular weight

Defining and Modifying Pseudocomponent Property Correlation Option Sets

Input Language for PC-PROP-OPT

```
PC-PROP-OPT    pcopsetname    base-pcopsetname    propkeyword    model  /  &
propkeyword    model  /  ...
```

Input Language Description for PC-PROP-OPT

Use the PC-PROP-OPT paragraph to construct a new pseudocomponent correlation option set from a base option set and to construct built-in correlations. (See Table 7.3 for the complete list of built-in correlations.)

pcopsetname ..... User-assigned name for new PC option set

base-pcopsetname..... Base option set name. Use any of the five built-in option sets from Table 7.2.

propkeyword ..... Keyword for property from Table 7.3

model ..... Name of correlation for property from Table 7.3

Table 7.3 Pseudocomponent Correlations

Property	Propkeyword	Model	Model Description
Molecular weight	MW	MWRZI	Riazi (1980)
		MWASPN	Tsang-ASPEN (1978)
		MWSTAR	Brule et al. (1982)
		MWKL	Kesler, Lee (1976)
		MWHS	Hariu, Sage (1969)
		MWUSR	User routine PCMWU
		MWRZAPI5	Riazi (1986)
		MWRZH	Riazi (1986), heavy petroleum
		HS-ASP	Hariu, Sage-ASPEN
Critical temperature	TC	TCRZI	Riazi (1980)
		TCASPN	Tsang-ASPEN (1978)
		TCSTAR	Brule et al. (1982)
		TCCAVT	Cavett (1962)
		TCKL	Kesler, Lee (1976)
		TCUSR	User routine PCTCU
		TCRZAPI5	Riazi (1986)
		TCTWU	Twu (1984)
		TCPR	Robinson-Peng (1978)
		TCWINN	Winn correlation
Critical pressure	PC	PCRZI	Riazi (1980)
		PCASPN	Tsang-ASPEN (1978)
		PCCAVT	Cavett (1962)
		PCKL	Kesler, Lee (1976)
		PCUSR	User routine PCPCU
		PCRZAPI5	Riazi (1986)
		PCTWU	Twu (1984)
		PCPR	Robinson-Peng (1981)
		PCWINN	Winn correlation
Critical volume	VC	VCRDL	Reidel (1954)
		VCSTAR	Brule et al. (1982)
		VCUSR	User routine PCVCU
		VCTWU	Twu (1984)
		VCEDMIS	Edmister (1988)
		VCKL	Kesler, Lee (1976)
Vapor pressure	PL	PLMB	Maxwell, Bonnell (1955)
		PLSWAP	Tsang-SWAP (1978)
		PLKL	Kesler, Lee (1980)
		PLUSR	User routine PCPLU
		BK-10	BK-10 model

continued

Table 7.3 Pseudocomponent Correlations (continued)

Property	Propkeyword	Model	Model Description
Ideal gas heat capacity	CPIG	CPIGKL	Kesler, Lee (1976)
		CPIGASPN	Tsang-ASPEN (1978)
		CPIGSTAR	Brule et al. (1982)
		CPIGCAVT	Cavett (1962)
		CPMM	Mathias, Monks (1982)
		CPIGUSR	User routine PCCPGU
		CPIGAPI	API hybrid
		CPIGSKL	Simplified Kesler Lee
Liquid molar volume	VL	VLRKT	Rackett (Spencer, 1972)
		VLCAVT	Cavett
		VLUSR	User routine PCVOLU
Enthalpy of vaporization	DHVL	DHVLVET	Vetere (1973)
		DHVLUSR	User routine PCDHVU
		DHVLKIST	Kistiakowsky (1923)
Acentric factor	OMEGA	OMEGADEF	Defining relation
		OMEGAKL	Kesler, Lee (1976)
		OMEGAUSR	User routine PCOMGU
		OMEGAPR	Robinson-Peng (1981)
		KL-ASPEN	Lee-Kesler, ASPEN
		OMGEDMIS	Edmister (1988)
Viscosity	MUL	MULWAT	Watson (1935)
		MULUSR	User routine PCMULU
BWR orientation parameter	BWRGMA	GMASTAR	Brule et al. (1982)
		GMAUSR	User routine PCBWRU
BWR critical temperature	TCBWR	TCSTAR	Brule et al. (1982)
		TCBWUSR	User routine PCBWRU
BWR critical volume	VCBWR	VCSTAR	Brule et al. (1982)
		VCBWUSR	User routine PCBWRU
Standard enthalpy of formation	DHFORM	DHFMZERO	Defaults to zero
		DHFMONT	Edmister (1988)
		DHFMUSR	User routine PCDHFU
		DHFMAPI	Edmister/API (1988)
Standard free energy of formation	DGFORM	DGFMZERO	Defaults to zero
		DGFMUSR	User routine PCDGFU
		DGFMONT	Edmister
RKS interaction parameters	RKSKIJ	API78	API, 3rd Ed.
		API87	API, 5th Ed.
		KIJUSR	User routine PCRKIU
Water solubility	WATSOL	WSOLASPN	ASPEN model
		KEROSENE	API, Kerosene line
		WSOLUSR	User routine PCWSLU
		WSOLAPI	API, procedure 9A1.5

Entering Properties for Pseudocomponents

Input Language for PC-PROP-DATA

```
PC-PROP-DATA
VAPOR-PRES   pcid   temp   vp  /  temp   vp  /  ...
VISCOSITY    pcid   temp   visc  /  temp   visc  /  ...
MOLE-SOLU    pcid   temp   wsol  /  temp   wsol  /  ...
```

Input Language Description for PC-PROP-DATA

Use the PC-PROP-DATA paragraph to enter vapor pressure, viscosity, and water solubility data for the user-defined pseudocomponents. Aspen Plus estimates these properties if they are not entered.

VAPOR-PRES Use to enter vapor pressure data for the user-defined pseudocomponent. Aspen Plus estimates vapor pressure, if it is not specified.

pcid ..... Pseudocomponent ID

temp ..... Temperature

vp ..... Vapor pressure

VISCOSITY Use to enter viscosity data for the user-defined pseudocomponent. Aspen Plus estimates viscosity, if it is not specified.

pcid ..... Pseudocomponent ID

temp ..... Temperature

visc ..... Viscosity

MOLE-SOLU Use to enter water solubility data for the user-defined pseudocomponent. Aspen Plus estimates water solubility, if it is not specified.

pcid ..... Pseudocomponent ID

temp ..... Temperature

wsol ..... Water solubility in mole fraction of water

Entering Petroleum Properties for Light End Components

Input Language for LE-PROP-DATA

```
LE-PROP-DATA
LE-PROP    propname    cid    value  /  cid    value  /  . . .
```

Input Language Description for LE-PROP-DATA

Use the LE-PROP-DATA paragraph to enter petroleum properties for light end components.

LE-PROP Use to petroleum properties for light end components.

propname ..... Name of the petroleum property (Table 7.1)

cid ..... Component ID

value ..... Value of the petroleum property for the component

8 Properties

This chapter discusses:

- Physical property methods.
- Physical property data.
- Property parameter estimation.
- CAPE-OPEN property packages.

Physical Property Methods

This section describes the input language used for specifying physical property methods. It discusses how to:

- Specify property option sets.
- Modify option sets.
- Use special property models.

Specifying Property Option Sets

Input Language for PROPERTIES

```
PROPERTIES          opsetname    keyword=value  /
                 opsetname    [sectionid-list]    keyword=value  / . . .
```

Optional keywords:

FREE-WATER SOLU-WATER HENRY-COMPS CHEMISTRY TRUE-COMPS

```
HENRY-COMPS    henryid    cid-list
NC-PROPS  cid    propname    modelname    [option-list]  /  . . .
```

Input Language Description for PROPERTIES

Use the PROPERTIES paragraph to specify option sets including free-water phase option sets, water solubility options, Henry's law component list IDs, chemistry IDs, and electrolyte simulation approach. You must enter at least one set of PROPERTIES specifications. The first set you enter becomes the default set for the entire flowsheet. Subsequent sets are optional and replace the default set for the sections that you list. You must also enter any option set used only at the individual block level.

opsetname..... Primary option set name

sectionid-list..... List of flowsheet section IDs

FREE-WATER..... Free-water phase option set name (Default=STEAM-TA)

SOLU-WATER..... Method for calculating the K-value of water in the organic phase. Use in conjunction with free-water calculations. (See Chapter 45.)

SOLU-WATER=0	Water solubility correlation is used. Vapor phase fugacity for water is calculated by the free-water phase option set.
SOLU-WATER=1	Water solubility correlation is used. Vapor phase fugacity for water is calculated by the primary option set.
SOLU-WATER=2	Water solubility correlation is used with a correction for unsaturated systems. Vapor phase fugacity for water is calculated by the primary option set.

	SOLU-WATER=3	Primary option set is used. This method is required for rigorous three-phase calculations. This method is not recommended for water-hydrocarbon systems unless water-hydrocarbon interaction parameters are available. (Default)
	SOLU-WATER=4	Same as SOLU-WATER=2, except water solubility limit is 1. Intended for VLE systems where the liquid phase is predominantly water.

HENRY-COMPS ..... Henry's law component list ID

CHEMISTRY..... Chemistry ID. (See Chapter 5.)

TRUE-COMPS..... True or apparent component approach. Use in electrolyte simulation.

TRUE-COMPS=YES	True component approach (Default)
TRUE-COMPS=NO	Apparent component approach. Chemistry ID is required.

Input Language Description for HENRY-COMPS

Use the HENRY-COMPS paragraph to identify lists of components that use Henry's law and infinite dilution normalization. You can have any number of HENRY-COMPS paragraphs, because different lists can apply to different blocks or flowsheet sections.

henryid ..... Henry's law component list ID

cid-list ..... List of component IDs

Input Language Description for NC-PROPS

Use the NC-PROPS paragraph to specify the physical property models and method options for each nonconventional component. You cannot change the specification for different sections or blocks.

cid..... Nonconventional component ID defined in NC-COMPS paragraph. (See Chapter 4.)

propname ..... Property name (ENTHALPY or DENSITY)

modelname..... Physical property model name. (See Table 8.1.)

option-list..... List of option codes corresponding to the calculation steps in the physical property model. Use only for special coal models. (See *Aspen Plus Physical Property Methods and Models*, Chapter 3.)

Table 8.1 Nonconventional Property Models

Property Name	Model Name	Parameter Requirements	Attribute Requirements
General Models†			
ENTHALPY	ENTHGEN	[DHFGEN]	GENANAL
DENSITY	DNSTYGEN	DENGEN	GENANAL
Special Models for Coal and Coal-Drived Materials†			
ENTHALPY	HCOALGEN	[BOIEC], [DLNGC], [GMLDC], [HCOMB], [HFC], [CP1C], [CP2C]	ULTANAL, PROXANAL, SULFANAL
DENSITY	DCOALIGT	[DENIGT]	ULTANAL, SULFANAL
	DCHARIGT	[DENIGT]	ULTANAL, SULFANAL

† See Aspen Plus Physical Property Methods and Models, Chapter 3, for detailed descriptions.

Modifying Option Sets

This section discusses:

- Using PROP-REPLACE to create or modify option sets.
- Using MP-ROUTE and SP-ROUTE to build your own routines.
- Using PROP-OPTIONS to create or modify option sets.

Using PROP-REPLACE to Create or Modify Option Sets

Input Language for PROP-REPLACE

To modify all option sets in a simulation:

```
PROP-REPLACE
PROP    propname    routeid
MODEL    modelname    [setno]    [OPCODES=opcode-list]
```

To modify a specified option set:

```
PROP-REPLACE    opsetname
PROP    propname    routeid
MODEL    modelname    [setno]    [OPCODES=opcode-list]
```

To create a new option set:

```
PROP-REPLACE    new-opsetname    base-opsetname
PROP    propname    routeid
MODEL    modelname    [setno]    [OPCODES=opcode-list]
```

Input Language Description for PROP-REPLACE

opsetname ..... Name of the option set that is to be modified. Do not modify SYSOP0 because it is used to initialize many unit operations based on Raoult's Law. Create a new option set instead.

new-opsetname ..... Name selected for the new option set

base-opsetname ..... Name of the option set to which the changes are applied

PROP

Use to enter the physical property name and route ID.

propname ..... Physical property name. Obtain from *Aspen Plus Physical Property Methods and Models*, Tables 4.1 and 4.2 for major and subordinate properties.

routeid ..... System route ID or route ID of a route you built using MP-ROUTE or SP-ROUTE

MODEL

Use to enter the new physical property model name, parameter data set number, and the model option code.

modelname ..... Physical property model name. Obtain model names from *Aspen Plus Physical Property Methods and Models*, Tables 4.21 and 4.22, or from the user physical property model name in *Aspen Plus User Models*, Chapter 6.
(See Note 1.)

setno ..... Parameter data set number. The model descriptions in *APrSystem Physical Property Methods and Models*, Chapter 3, indicate which model parameters can have multiple sets of data. (Default=1) (See Note 2.)

opcode-list ..... List of model option codes. (See *APrSystem Physical Property Methods and Models*, Chapter 3.)

Notes

1 Property models in Aspen Plus are divided into two categories:

- Equation-of-state models
- Non-equation-of-state models

If you specify this model type in PROP-REPLACE	The model will be used for all properties that were calculated by
Equation-of-state	An equation-of-state model in the base option set
Non-equation-of-state	A non-equation-of-state model in the base option set

An equation-of-state has different model names for mixture and pure component properties. When you replace an equation-of-state model, enter both names.

2 When you enter a *setno* greater than 1 for a model, Aspen Plus creates a new data set for all parameters for that model that can take more than one data set. These parameters are indicated with an X in the Multiple Data Set (MDS) column. (See *APrSystem Physical Property Methods and Models*, Chapter 3.) Then you can use PROP-DATA paragraphs to specify parameter values for the data set. Any unspecified parameters default to the values for the previous data set number. For example, values for data set 2 default to the values established for data set 1.

Using MP-ROUTE and SP-ROUTE to Build Your Own Routes

Input Language for MP-ROUTE and SP-ROUTE

To build major property routes:

```
MP-ROUTE  new-routeid  propname  methodcode  base-routeid
MODEL  modelname  [setno]  [OPCODES=opcode-list]
MPROP  propname  routeid
SPROP  propname  routeid
OPCODES  method-opcode-list
```

To build subordinate property routes:

```
SP-ROUTE  new-routeid  propname  methodcode  base-routeid
MODEL  modelname  [setno]  [OPCODES=opcode-list]
MPROP  propname  routeid
SPROP  propname  routeid
OPCODES  method-opcode-list
```

Input Language Description for MP-ROUTE and SP-ROUTE

new-routeid ..... New route ID. An 8-character route identifier.

propname ..... Name of the major or subordinate property. Obtain from *Aspen Plus Physical Property Methods and Models*, Tables 4.1 and 4.2.

methodcode ..... Method to use in the property calculation. See the route structure in *Aspen Plus Physical Property Methods and Models*, Tables 4.4 through 4.20, for appropriate method code.

base-routeid ..... Base route ID. If you specify a base route ID, it will be modified using the information you give in the MODEL, MPROP, SPROP, or OPCODES sentences. If you specify an asterisk (*), Aspen Plus will build the entire route. The base route can be either a system built-in route, or a route you create using another MP-ROUTE or SP-ROUTE paragraph.

MODEL

Use to specify the physical property model name, parameter data set number, and model option code.

modelname ..... Physical property model name. Obtain from *Aspen Plus Physical Property Methods and Models*, Tables 4.21 and 4.22.

setno ..... Optional data set number (Default=1)

OPCODES ..... List of model option codes. (See *APrSystem Physical Property Methods and Models*, Chapter 3.)

MPROP

Use to specify the property name and route ID of other major properties used in building the new route. The route can be a system built-in route, or a route you created in another MP-ROUTE paragraph.

propname ..... Name of major property. Obtain from *Aspen Plus Physical Property Methods and Models*, Table 4.1.

routeid ..... Route ID

SPROP

Use to specify the property name and route ID of other subordinate properties to be used in building the new route. The route specified using SPROP can be a system built-in route or a route you created in another SP-ROUTE paragraph.

propname ..... Name of subordinate property. Obtained from *Aspen Plus Physical Property Methods and Models*, Table 4.2.

routeid ..... Route ID

OPCODES

Use to enter method option codes. The only application of these codes is for specifying the number of integration points for numerical integration of volume with respect to pressure. For example, this is used in calculating subordinate property PHILPC. See the route structure in *Aspen Plus Physical Property Methods and Models*, Tables 4.4 through 4.20. The integration uses a Gaussian quadrature formula with up to five points. The default (one point) is satisfactory unless the pressure is very high.

method-opcode-list..... List of method option codes

Using PROP-OPTIONS to Create or Modify Option Sets

Input Language for PROP-OPTIONS

To create a new option set:

```
PROP-OPTIONS  new-opsetname  *  propname  routeid / ...
```

To create a new option set by modifying an existing option set:

```
PROP-OPTIONS  new-opsetname  base-opsetname  propname  routeid / ...
```

Input Language Description for PROP-OPTIONS

new-opsetname ..... Name selected for the new option set

base-opsetname ..... Name of the option set to which the changes are applied

propname ..... Name of the major property. Obtain from *Aspen Plus Physical Property Methods and Models*, Table 4.1.

routeid ..... Route ID of the major property. The route ID can be either a built-in major property route, or a major property route you created using an MP-ROUTE paragraph.

Using Special Property Models

Use the physical property models discussed in this section for certain special applications instead of the built-in models.

This section describes the special models for:

- Petroleum mixtures.
- Transport property.
- Liquid density.

Special Petroleum Mixtures Models

The following table describes physical property models, based on API-recommended procedures.

Use this model	To calculate
VL2API	Liquid molar volume
MUL2API	Liquid viscosity
SIG2API	Liquid surface tension

See *APrSystem Physical Property Methods and Models*, Chapter 3, for more information.

To use these models, enter the INSERT paragraph:

Input Language

```
INSERT   *   API   [opsetname]
```

Input Language Description

opsetname..... Name of the option set in which the special models are used. If you do not enter *opsetname*, Aspen Plus uses the special models in all option sets in the simulation.

By default, Aspen Plus uses these models in option sets: PENG-ROB, RK-SOAVE, LK-PLOCK, BK10, BWR-LS, CHAO-SEA, and GRAYSON.

Special Transport Property Models

The physical property models MUL2TRAP, MUL0TRAP, MUV2TRAP, MUV0TRAP, KL2TRAP, KL0TRAP, KV2TRAP and KV0TRAP described in *APrSystem Physical Property Methods and Models*, Chapter 3, are recommended for calculating viscosity and thermal conductivity for gas-hydrocarbon mixtures. You can use these models for both vapor and liquid-phase properties. The mixture should contain only hydrocarbons and light gases such as carbon-dioxide. These models are not applicable to polar and associating components.

These models, known as TRAPP, are based on the methods recommended by NBS (Ely, J. F. and H. J. M. Hanley, *Ind. Eng. Chem. Fundam, 20*, 323 (1981); *ibid*., *22*, 90 (1983)). The authors reported the accuracy of the viscosity models to be 8.4% and 7.0% for pure component and binary mixtures, respectively. For thermal conductivity, the reported accuracy is 6.6% and 6.8%.

To use these models, enter the INSERT paragraph:

Input Language

```
INSERT   *   TRAPP   [opsetname]
```

Input Language Description

opsetname..... Name of the option set in which the special models are used. If you do not enter *opsetname*, Aspen Plus uses the special models in all option sets in the simulation.

By default Aspen Plus uses the TRAPP models in option sets PR-BM and RKS-BM.

Special Liquid Density Model

The physical property models VLMX22 and VL06 are recommended for calculating saturated and compressed liquid volumes for organic mixtures and certain inorganic gases such as hydrogen sulfide. (See *Aspen Plus Physical Property Methods and Models*, Chapter 3.) Hankinson and Thomson (*AIChE J., 25*, 653 (1979)) and Thomson et al. (*ibid*, *28*, 671 (1982)) developed the COSTALD method. The authors reported parameters for over 400 compounds. (See Reid et al., *The Properties of Gases and Liquids,* 4th Edition, Chapter 3, 1987.) The COSTALD method is an improvement over the Rackett method, which is used in all the activity-coefficient-based option sets. In addition, the COSTALD method is applicable to the compressed liquid states.

To use the COSTALD model, enter the INSERT paragraph:

Input Language

```
INSERT   *   COSTLD   [opsetname]
```

Input Language Description

opsetname..... Name of the option set in which the special models are used. If you do not enter *opsetname*, Aspen Plus uses the special models in all option sets in the simulation.

Physical Property Data

This section discusses:

- Databanks.
- Built-in equation-of-state parameters.
- Entering physical property data.
- Tabular and polynomial models and data.
- UNIFAC models.

Databanks

This section describes how to:

- Retrieve data from the databanks.
- Control the databank search order.

Retrieving Data from Aspen Plus System Databanks

Input Language for DATABANKS

```
DATABANKS    password  /  ...
```

Input Language Description for DATABANKS

password ..... Databank password. Obtain password from *Aspen Plus Physical Property Data*, Table 1.1. The order in which you enter the password does not determine the order in which the data are retrieved. Use the PROP-SOURCES paragraph to specify the order of data retrieval.

Retrieving Data from In-House Databanks

Input Language for IN-HOUSE-DATA

IN-HOUSE-DATA $\left\{ \begin{matrix} \text{PCD} \\ \text{SOLIDS} \\ \text{AQUEOUS} \\ \text{BINARY} \end{matrix} \right\} = \left\{ \begin{matrix} \text{YES} \\ \text{NO} \end{matrix} \right\}$

Input Language Description for IN-HOUSE-DATA

PCD Search the in-house PCD databank. An operating system error will occur if you specify PCD=YES, and an in-house PCD databank is not installed.

PCD=YES ..... Searches the in-house pure component databank

PCD=NO..... Does not search the in-house pure component databank

SOLIDS Search the in-house SOLIDS databank. An operating system error will occur if you specify SOLIDS=YES, and an in-house SOLIDS databank is not installed. You must specify the Aspen Plus system SOLIDS databank in the DATABANKS paragraph to retrieve data from the in-house SOLIDS databank.

SOLIDS=YES Searches the in-house SOLIDS databank before the Aspen Plus system SOLIDS databank

SOLIDS=NO Does not search the in-house SOLIDS databank

AQUEOUS Search the in-house AQUEOUS databank. An operating system error will occur if you specify AQUEOUS=YES, and an in-house AQUEOUS databank is not installed. You must specify the Aspen Plus system AQUEOUS databank in the DATABANKS paragraph to retrieve data from the in-house AQUEOUS databank.

AQUEOUS=YES Searches the in-house AQUEOUS databank before the Aspen Plus system AQUEOUS databank

AQUEOUS=NO Does not search the in-house AQUEOUS databank

BINARY Search the in-house BINARY databank. An operating system error will occur if you specify BINARY=YES, and an in-house BINARY databank is not installed. You must specify the Aspen Plus system BINARY databank in the DATABANKS paragraph to retrieve data from the in-house BINARY databank.

BINARY=YES Searches the in-house BINARY databank before the Aspen Plus system BINARY databank

BINARY=NO Does not search the in-house BINARY databank

Using PROP-SOURCES to Control Databank Search Order

Input Language for PROP-SOURCES

To specify a global search order:

```
PROP-SOURCES
GLOBAL    password    [COMPS=cid-list]    [PAIRS=pairid-list]  / ...
```

To override global search order:

```
PROP-SOURCES
GLOBAL    password    [COMPS=cid-list]    [PAIRS=pairid-list]  / ...
LOCAL     password    [COMPS=cid-list]    [PAIRS=pairid-list]  / ...
RETRIEVE    paramname  / ...
```

Input Language Description for PROP-SOURCES

GLOBAL Used to define the global search order for the data retrieval, unless the LOCAL and RETRIEVE sentences override it for individual properties. If you do not specify the GLOBAL sentence, Aspen Plus searches the system databanks in the following order: ASPENPCD, FLOWTRAN, SOLIDS, AQUEOUS, BINARY, COMBUST, PURECOMP, and INORGANIC.

The in-house databanks will be searched before the Aspen Plus databanks, if you do not specify the GLOBAL sentence. In this case the search order is: in-house PCD (INHSPCD), in-house SOLIDS (INHSSOL), in-house AQUEOUS (INHSAQUS), in-house binary (INHSBIN), ASPENPCD, SOLIDS, AQUEOUS, and BINARY.

You must enter either the GLOBAL sentence or the LOCAL and RETRIEVE sentences for user's databanks.

password ..... Password assigned when the databank was created. The search order for data retrieval will be the order in which the passwords are specified.

cid-list ..... List of component IDs (Default=ALL)

pairid-list ..... List of component pair IDs of the form (C1 C2) (C2 C4) . . . (Default=ALL pairs)

LOCAL, RETRIEVE

You must enter the LOCAL and RETRIEVE sentences as a pair. They specify exceptions to the GLOBAL sentences for properties listed in the RETRIEVE sentence and for components listed in the corresponding LOCAL sentence.

password ..... Password assigned when the databank was created. The search order for data retrieval will be the order in which the passwords are specified.

cid-list ..... List of component IDs (Default=ALL)

pairid-list ..... List of component pair IDs of the form (C1 C2) (C2 C4) . . . (Default=ALL pairs)

paramname ..... Parameter name

Built-in Equation-of-State Parameters

Input Language for MODEL-PARAMETER

To search model parameter tables that are not searched automatically:

```
MODEL-PARAMETER    tablename    [setno] / ...
```

To suppress search of model parameter tables:

```
MODEL-PARAMETER    NOtablename
```

Input Language Description for MODEL-PARAMETER

tablename ..... Name of table containing model parameters. Table names and retrieved parameters for each equation-of-state model are listed in the following table.

setno ..... Data set number to which data retrieved from the table are assigned (Default=1)

NOtablename ..... Name of table that is not to be searched, prefixed by NO

Table name	Equation-of-state	Option set	Retrieved parameters
APIRKS	Redlich-Kwong-Soave	RKS-BM	RKSKIJ†
ESCSTBWR	BWR-Lee-Starling	BWR-LS	BWRKV††, BWRKT††, TCBWR, VCBWR, BWRGMA
ESHOC†††	Hayden O'Connell	WILS-HOC, NRTL-HOC, UNIQ-HOC, UNIF-HOC	HOCETA
ESLKP	Lee-Kesler-Plöcker	LK-PLOCK	LKPKIJ††, TCLKP, PCLKP, VCLKP, OMGLKP
ESPR	Peng-Robinson, Boston-Mathias alpha function	PR-BM	PRKIJ††, TCPR, PCPR, OMGPR
ESPRSTD†††	Peng-Robinson, standard literature version	PENG-ROB	PRKIJ††, TCPRS, PCPRS, OMGPRS
ESRKS	Redlich-Kwong-Soave, Boston-Mathias alpha function	RKS-BM	RKSKIJ††, TCRKS, PCRKS, OMGRKS
ESRKSTD†††	Redlich-Kwong-Soave, standard literature version	RK-SOAVE	RKSKIJ††, TCRKSS, PCRKSS, OMRKSS

† Binary parameters recommended by API.

†† Binary parameters. Other parameters are pure component parameters from the same data source for consistency.

††† The table is searched by default.

Entering Physical Property Data

Input Language for PROP-DATA

```
PROP-DATA
PROP-LIST   paramname   [setno] / ...
PVAL   cid   value-list / value-list / ...
PROP-LIST   paramname   [setno] / ...
BPVAL   cid1   cid2   value-list / value-list / ...

COMP-LIST   cid-list
CVAL   paramname   setno   1   value-list
COMP-LIST   cid-list
BCVAL   paramname   setno   1   cid1   value-list /  1   cid1   value-list / ...
```

Input Language Description for PROP-DATA

PROP-LIST Use to enter parameter names and data set numbers. (See Notes 1 and 2.)

paramname ..... Parameter name (See Note 3.)

setno ..... Data set number (default is 1). For *setno* > 1, see Note 4.

PVAL Use to enter PROP-LIST parameter values.

cid..... Component ID

value-list ..... List of parameter values. Enter one value for each property element. (See Note 5.)

BPVAL Use to enter PROP-LIST binary parameter values.

cid1..... Component ID of first component of binary pair

	cid2	Component ID of second component of binary pair
	value-list	List of parameter values. Enter one value for each property element. (See Note 5.)
COMP-LIST	Use to enter component IDs. (See Note 1.)	
	cid-list	List of component IDs
CVAL	Use to enter COMP-LIST parameter values.	
	paramname	Parameter name (See Note 3.)
	setno	Data set number (required). For *setno* > 1, see Note 4.
	value-list	List of parameter values. Enter one value for each component in the *cid-list*. (See Note 5.)
BCVAL	Use to enter COMP-LIST binary parameter values.	
	paramname	Parameter name (See Note 3.)
	setno	Data set number (required). For *setno* > 1, see Note 4.
	cid1	Component ID of first component of binary pair
	cid2	Component ID of second component of binary pair
	value-list	List of parameter values. Enter one value for each component in the *cid-list*. (See Note 5.)

Notes

1 Any number of PVAL or BPVAL statements can follow an associated PROP-LIST statement. Any number of CVAL or BCVAL statements can follow an associated COMP-LIST statement.

2 If a parameter consists of a vector of values, you must use the PROP-LIST form to enter them. You can truncate the vector when entering values. Defaults will be used for the truncated values.

3 The allowed parameters are ones defined by the models in the property methods declared in the simulation. The model descriptions in *Physical Property Methods and Models*, Chapter 3 show the parameters for each model. In addition, certain parameters may always be specified and are useful for specifying non-databank components or augmenting the data available in databanks. These parameters are listed in the table below.

4 For *setno* > 1, you must also specify the data set number in a new option set defined using the PROP-REPLACE paragraph, or in new routes defined using the MP-ROUTE and SP-ROUTE paragraphs. (See Using PROP-REPLACE to Create or Modify Option Sets, this chapter.)

5 You can include an IN-UNITS sentence as the first sentence of a PROP-DATA paragraph. (See Chapter 3.) The model descriptions in *Physical Property Methods and Models*, Chapter 3 show the required units keywords for each parameter. For certain parameters, the temperature units are always absolute. In these cases, Aspen Plus assumes Rankine or Kelvin temperature units, even if Fahrenheit or Centigrade units are in effect for the PROP-DATA paragraph. The table below shows the units for other parameters which can be used in PROP-DATA.

Parameters Always Allowed in PROP-DATA

Propname	Description	Units keyword
API	Standard API gravity at 60°F	—
ATOMNO	Vector of atomic numbers of atoms in a molecule †	—
CHARGE	Ionic charge	—
CPIG	Ideal gas heat capacity coefficients	††
CPIGDP	DIPPR ideal gas heat capacity coefficients	††
DHFORM	Standard heat of formation; ideal gas at 25°C	MOLE-ENTHALPY
DHVLWT	Watson heat of vaporization parameters	††
DGFORM	Standard Gibbs free energy of formation; ideal gas at 25°C	MOLE-ENTHALPY
MW	Molecular weight	—
NOATOM	Vector of numbers of atoms of each type in a molecule †	—
OMEGA	Pitzer acentric factor	—
PC	Critical pressure	PRESSURE
PLXANT	Extended Antoine vapor pressure coefficients	††
S025E	Sum of absolute entropy of the elements of a compound at 25°C	MOLE-ENTROPY
SG	Standard specific gravity at 60°F	—
TB	Normal boiling point	TEMPERATURE
TC	Critical temperature	TEMPERATURE
TFP	Normal freezing point	TEMPERATURE
VLSTD	Standard liquid volume at 60°F	MOLE-VOLUME
WATSOL	Water solubility correlation coefficients	††
ZC	Critical compressibility factor	—

† Use ATOMNO and NOATOM to define the chemical formula of a molecule. These are used to compute molecular weight, and in RGibbs.

†† See chapter 3 of *Physical Property Methods and Models* for details of meanings and units, as indicated below.
For CPIG and CPIGDP, see Ideal Gas Heat Capacity/DIPPR.
For DHVLWT see Watson Equation.
For PLXANT, see Extended Antoine/Wagner/IK-CAPE.
For WATSOL see Water Solubility.

Tabular and Polynomial Models and Data

This section describes the input language for:

- Specifying tabular and polynomial models.
- Entering tabular and polynomial data.

TABPOLY Models

To use tabular data or polynomial coefficients for any property listed in Table 8.2, you must use the PROP-REPLACE paragraph. Aspen Plus then calculates these properties, using the tabular data or the polynomial coefficients you entered. (See Entering TABPOLY Data, this chapter.) If you do not provide data for some components, Aspen Plus will use the property models for the ideal option set, SYSOP0, for those components. Aspen Plus calculates mixture properties using mole-fraction average ideal mixing expressions.

The polynomial expression used for all the properties in Table 8.2 is:

$$\left\{ \begin{matrix} propname \\ \ln(propname) \end{matrix} \right\} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + \frac{a_5}{T} + \frac{a_6}{T^2} + \frac{a_7}{\sqrt{T}} + a_8 \ln T$$

Input Language

```
PROP-REPLACE    [opsetname] / ...
TABPOLY-MODEL    propname / ...
```

Input Language Description

opsetname..... Name of option set to be modified (Default=all option sets)

propname ..... Name of property whose calculation method will be replaced by a TABPOLY model. (See Table 8.2.)

Table 8.2 TABPOLY Properties

Propname	Description	Polynomial paramname	Units keyword
PHIV†	Pure component vapor fugacity coefficient	PHIVPY	—
PHIL†	Pure component liquid fugacity coefficient	PHILPY	—
PHIVMX†	Vapor fugacity coefficient for a component in a mixture	PHVMPY	—
PHILMX†	Liquid fugacity coefficient for a component in a mixture	PHLMPY	—
PL†	Vapor pressure	PLPY	PRESSURE
KVL†	Vapor-liquid K-value	KVLPY	—
VV	Vapor volume	VVPY	MOLE-VOLUME††
VL	Liquid volume	VLPY	MOLE-VOLUME††
MUV	Vapor viscosity	MUVPY	VISCOSITY
MUL†	Liquid viscosity	MULPY	VISCOSITY
KV	Vapor thermal conductivity	KVPY	THERMAL-CONDUCTIVITY
KL	Liquid thermal conductivity	KLPY	THERMAL-CONDUCTIVITY
DVMX	Vapor diffusion coefficient	DVMXPY	DIFFUSIVITY
DLMX	Liquid diffusion coefficient	DLMXPY	DIFFUSIVITY
SIGL	Surface tension	SIGLPY	SURFACE-TENSION
HNRY†	Henry's constant	HNRYPY	PRESSURE
HIG	Ideal gas enthalpy	HIGPY	MOLE-ENTHALPY††
HV	Vapor enthalpy	HVPY	MOLE-ENTHALPY††
DHV	Vapor enthalpy departure	DHVPY	MOLE-ENTHALPY††
HL	Liquid enthalpy	HLPY	MOLE-ENTHALPY††
DHL	Liquid enthalpy departure	DHLPY	MOLE-ENTHALPY††
DHVL	Enthalpy of vaporization	DHVLPY	MOLE-ENTHALPY††
SIG†††	Ideal gas entropy	—	MOLE-ENTROPY††
SV	Vapor entropy	SVPY	MOLE-ENTROPY††
DSV	Vapor entropy departure	DSVPY	MOLE-ENTROPY††
SL	Liquid entropy	SLPY	MOLE-ENTROPY††
DSL	Liquid entropy departure	DSLPY	MOLE-ENTROPY††
GIG†††	Ideal gas free energy	—	MOLE-ENTHALPY††
GV	Vapor free energy	GVPY	MOLE-ENTHALPY††
DGV	Vapor free energy departure	DGVPY	MOLE-ENTHALPY††
GL	Liquid free energy	GLPY	MOLE-ENTHALPY††
DGL	Liquid free energy departure	DGLPY	MOLE-ENTHALPY††

† The tabular model uses the logarithmic transformation of the property to interpolate; the polynomial model is the logarithmic form of the equation.

†† See Note 6.

††† Valid for REF-DATA sentences only.

Entering TABPOLY Data

In the PROP-DATA paragraph you must enter a TABPOLY-DATA sentence for every TABPOLY model, except entropy and Gibbs free energy. (See Note 1.)

Use these sentences	To enter
TABVAL	Tabular data for a component
PROP-LIST and PVAL	Polynomial coefficients
REF-DATA and REF-PRES	Optional reference data

Aspen Plus uses SYSOP0 physical property models for the components for which neither tabular nor polynomial data are entered.

Input Language

```
PROP-DATA
TABPOLY-DATA    propname    [keyword=value]
```

Keywords for tabular data:

TAB-BASIS TAB-REF

Keywords for polynomial coefficients:

POLY-BASIS POLY-REF

```
TABVAL   cid   1   temp   value / temp   value / ...

PROP-LIST   paramname
PVAL   cid   values

REF-DATA   propname   1   cid   temp   value / cid   temp   value / ...
REF-PRES   propname   1   cid   pres / cid   pres / ...
```

Input Language Description

TABPOLY-DATA

Identifies the name of the property and specifies whether the data are on a mass or mole basis, and whether the data will be adjusted. Use TAB-BASIS and TAB-REF when entering tabular data. For polynomial coefficients, use POLY-BASIS and POLY-REF.

propname ..... Property name. (See Table 8.2.)

TAB-BASIS..... Basis for tabular data. You can use only one basis for all tabular data for a given property.

TAB-BASIS=MOLE	Mole basis (Default)
TAB-BASIS=MASS	Mass basis (See Note 6.)

TAB-REF..... Thermodynamic reference state for enthalpy, entropy, and Gibbs free energy. (See Note 1.) If you do not provide the reference state in the REF-DATA sentence for TAB-REF=1 and TAB-REF=2, the Aspen Plus reference state will be used. (See Note 2.) TAB-REF values can be different for different components.

TAB-REF=0	Tabular data are used as you entered them. They are not adjusted to any reference state. If you enter tabular data for both vapor and liquid enthalpies, make sure they are based on the same reference state. (Default)
TAB-REF=1	Tabular data are adjusted to the reference state given in the REF-DATA sentence.

	TAB-REF=2	The same as TAB-REF=1, except that heat capacity data are entered instead of enthalpy data.

POLY-BASIS..... Basis for polynomial data. You can use only one basis for all polynomial data for a given property.

POLY-BASIS=MOLE	Mole basis (Default)
POLY-BASIS=MASS	Mass basis (See Note 6.)

POLY-REF..... POLY-REF is similar to TAB-REF, except only one value of POLY-REF can be used for a given property for all components. Use POLY-REF for polynomial coefficients.

TABVAL

Use to enter tabular data. Any number of TABVAL sentences can follow their associated TABPOLY-DATA sentence. You must enter the values in ascending order of temperature.

cid..... Component ID

temp ..... Temperature (in ascending order)

value..... Property value

PROP-LIST

Use to enter the polynomial parameter name.

paramname ..... Polynomial parameter name (See Table 8.2.)

PVAL

Use to enter polynomial parameter values. Any number of PVAL statements can follow an associated PROP-LIST statement.

cid..... Component ID

values ..... Polynomial coefficient values. (See Note 5.) If you truncate the vector, defaults will be used for the truncated values.

REF-DATA

Use to define the thermodynamic reference state. Applies to enthalpy, entropy, and Gibbs free energy only. (See Note 2.) The reference values must be at the same temperature in a given phase.

propname ..... Property name (See Table 8.2.)

cid..... Component ID

temp ..... Reference temperature

value..... Reference property value

REF-PRES

Use to specify reference pressures for vapor-liquid K-values, Gibbs free energies, or entropies. Calculated values are adjusted to the actual pressure. (See Note 3.)

propname ..... Property name (See Table 8.2.)

cid..... Component ID

pres ..... Reference pressure (pressure of the data)

Notes

1 If you enter vapor enthalpy data (HV), you should also enter ideal gas enthalpy data (HIG), to ensure consistency. If you enter enthalpy, entropy and Gibbs free energy, make sure they are consistent (G = H - TS). If you specify your own reference state, TAB-REF=1 or 2, or POLY-REF=1 or 2, and enter the reference values using REF-DATA, you must enter reference values for two of the three properties. If you do not supply reference values, the Aspen Plus reference state of elements in their standard state at 25ºC and 1 atm will be used.

If you entered only the enthalpy data (or equivalently, the heat capacity data) and specified the name of the additional properties to be generated using the PROP-REPLACE paragraph, Aspen Plus calculates entropy and Gibbs free energy automatically. For example, if you want Aspen Plus to generate liquid entropy from liquid enthalpy data, use:

```
PROP-REPLACE
TABPOLY-MODEL    HL  /  SL
```

In this case, you cannot use TAB-REF=0 or POLY-REF=0.

In order for Aspen Plus to generate entropy and Gibbs free energy from enthalpy data, the reference values for two of the three properties must be known. They can be obtained by either:

- System default, which uses the Aspen Plus reference state. The parameter values for DHFORM, DGFORM, PLXANT, and DHVLWT (or DHVLDP) must be available in the databanks or must be supplied. The REF-DATA sentence is not used.
- Using REF-DATA sentences to specify the reference values for two of the three properties. The reference values must be at the same temperature in a given phase.

2 For simulations with no chemical reaction, you can choose the reference states arbitrarily. For simulations with chemical reaction, the reference states must include the standard heat of formation for all components undergoing reaction. For simulations with equilibrium reactions, the reference states must include the standard Gibbs free energy of formation for all components undergoing reaction. Equilibrium reactions are modeled by the:

- REQUIL and RGIBBS reactor models. (See Chapter 19.)
- RADFRAC distillation models using the REACTIONS paragraph. (See Chapters 6 and 15.)

3 Aspen Plus adjusts vapor-liquid K-values, Gibbs free energies, and entropies for the effect of pressure using the following relationships:

$$K(T, P) = (Pref/P)\, K(T, Pref)$$

$$s(T, P) = s(T, Pref) - R \ln (P/Pref)$$

$$g(T, P) = g(T, Pref) + RT \ln (P/Pref)$$

Where:

Pref	=	Reference pressure
P	=	Actual pressure
T	=	Temperature
K(T, Pref)	=	K-value that you entered at the reference pressure
s(T, Pref)	=	Entropy that you entered at the reference pressure
g(T, Pref)	=	Gibbs free energy that you entered at the reference pressure

For K-value, Aspen Plus does not adjust for the pressure effect unless you supply the reference pressure in a REF-PRES sentence. The only time it is valid to enter no reference pressure is when the pressure range of the simulation matches that of the data.

If you use the Aspen Plus thermodynamic reference state for entropy and Gibbs free energy, Aspen Plus always performs an adjustment for the pressure effect using Pref=101325 N/m^2. If you do not use the Aspen Plus reference state, Aspen Plus adjusts for the pressure effect only if you supply the reference pressure in a REF-PRES sentence.

4 You can include an IN-UNITS sentence as the first sentence of a PROP-DATA paragraph for both tabular and polynomial data. See Chapter 3. Table 8.2 shows the units keyword for each property.

5 The polynomial model has the form:

$$\left\{ \begin{matrix} propname \\ \ln(propname) \end{matrix} \right\} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + \frac{a_5}{T} + \frac{a_6}{T^2} + \frac{a_7}{\sqrt{T}} + a_8 \ln T$$

Where a_9 and a_{10} are the lower and upper temperature limits respectively for the correlation. Linear extrapolation is performed outside this range. The coefficients a_2 through a_8 default to zero. The lower limit a_9 defaults to 0 K. The upper limit a_{10} defaults to 1000 K. The units keywords used to convert the coefficients are TEMPERATURE and the units keyword given for each property in Table 8.2. If a_5, a_6, a_7, or a_8 is non-zero, Aspen Plus assumes absolute temperature units for all parameters except a_9 and a_{10}.

6 If your data are on a mass basis, use the MOLE form of the units keyword, as shown in Table 8.2. Also use a TAB-BASIS=MASS or POLY-BASIS=MASS specification in the TABPOLY-DATA sentence. For example, if tabular enthalpy data will be entered as cal/gm, then:

- The IN-UNITS specification should include MOLE-ENTHALPY=CAL/MOL
- The TABPOLY-DATA specification should include TAB-BASIS=MASS

UNIFAC

This section describes the input language for using UNIFAC models. Aspen Plus contains five UNIFAC models, as shown in Table 8.3.

Table 8.3 UNIFAC Models in Aspen Plus

Model Name	Used in Option Sets	Parameter Name for Structure Information	Parameter Name for Group Area/Volume/ Binary Parameter
UNIFAC, Revision 5	UNIFAC, UNIF-LL, UNIF-HOC, SR-POLAR	UFGRP	GMUFR, GMUFQ, GMUFB
UNIFAC, Revision 4	—	UFGRP	GMUFR, GMUFQ, GMUFB4
UNIFAC, Revision 3	—	UFGRP	GMUFR, GMUFQ, GMUFB
Modified UNIFAC, Dortmund	UNIF-DMD	UFGRPD	GMUFDR, GMUFDQ, UNIFDM
Modified UNIFAC, Lyngby	UNIF-LBY	UFGRPL	GMUFLR, GMUFLQ, UNIFLB

The following input language is shown for the UNIFAC model, Revision 5. The input language for other UNIFAC models is analogous.

Input Language

To supply structural information for components:

```
PROP-DATA
PROP-LIST   UFGRP
PVAL   cid   groupno   noccur   groupno   noccur ...
```

To identify groups or to introduce new functional groups:

```
GROUPS   gid   groupno / ...
```

To enter vapor-liquid group parameters, for option sets UNIFAC, UNIF-HOC, and SR-POLAR:

```
PROP-DATA
PROP-LIST   GMUFQ / GMUFR
PVAL   gid   value / value

PROP-LIST   GMUFB
BPVAL   gid1   gid2   value
```

To enter liquid-liquid group parameters, for UNIF-LL:

```
PROP-DATA
PROP-LIST   GMUFQ   2 / GMUFR   2
PVAL   gid   value /  value

PROP-LIST   GMUFB   2
BPVAL   gid1   gid2   value
```

Input Language Description

cid..... Component ID

groupno ..... Group number. The group numbers for built-in groups are listed in *Aspen Plus Physical Property Data*, Tables 3.12 and 3.13. A user-defined group can use any *groupno* not listed in these tables. GMUFQ and GMUFR must be supplied or estimated for user-defined groups. If a user-defined group number falls within a built-in main group, the interaction parameters GMUFB will default to liquid-liquid main group values, if available, for UNIF-LL, and to vapor-liquid main group values for UNIFAC, UNIF-HOC, and SR-POLAR.

noccur..... Number of occurrences of a group in the molecular structure of a component. There is a limit of six groupno-noccur pairs for each component.

gid ..... Group ID

value..... Parameter value

gid1 ..... Group ID of first group of group pair

gid2 ..... Group ID of second group of group pair

Property Parameter Estimation

This section describes the input language used for property parameter estimation. It discusses how to:

- Specify parameters to be estimated.
- Define molecular structure.
- Enter experimental data.
- Use report options.
- Define user property parameters.

Specifying Parameters to be Estimated

Input Language for ESTIMATE

```
ESTIMATE    [option]
```

To estimate pure component constants:

```
propname    cid    method-name  /  [cid]    method-name  /  ...
```

To estimate temperature-dependent property correlation parameters:

```
propname    cid    method-name    keyword=value
```

Optional keywords:

TLOWER TUPPER DATA WEIGHT

To estimate binary parameters:

```
propname    cid1    cid2    method-name    [TEMP=value-list]
```

To estimate UNIFAC group parameters:

```
propname    gid    method-name  /  gid    method-name  /  ...
```

Input Language Description for ESTIMATE

option ..... **ALL** Estimates all missing parameters (Default)

ONLY Estimates only parameters specified using *propname* sentences

propname Property from the table in *Aspen Plus User Guide*, Chapter 30, "What Property Parameters can Aspen Plus Estimate" for which parameters are to be estimated. When *option*=ALL, Aspen Plus will use default methods for properties and components not listed in *propname* sentences.

cid..... Component ID

ALL All components

method-name ..... Method from *Aspen Plus User Guide*, Chapter 30, to be used in estimating parameters.

TLOWER ..... Lower temperature limit for temperature-dependent property correlations. (Default=TB for liquid properties, 298 K for vapor properties)

TUPPER ..... Upper temperature limit for temperature-dependent property correlations. (Default=TC for liquid properties, 1100 K for vapor properties)

DATA ..... Indicates whether experimental data should be used. (See Entering Experimental Data, this chapter.) Not used when *method-name*=DATA. To determine parameters from experimental data alone, specify *method-name*=DATA.

DATA=YES	Aspen Plus combines experimental data entered in PCES-PROP-DATA paragraphs with estimated values to determine the best correlation parameters
DATA=NO	Experimental data are not used (Default)

WEIGHT ..... Weighting factor for experimental data. Use when DATA=YES. The weighting factor for the estimated values is set to 1.0. Do not use when *method-name*=DATA. (Default=2.0)

cid1 ..... Component ID of first component in binary pair

ALL	All components

cid2 ..... Component ID of second component in binary pair

ALL	All components

TEMP ..... List of temperatures for which infinite dilution activity coefficients are estimated (Default=25°C)

gid ..... UNIFAC group ID defined in GROUPS paragraph

Defining Molecular Structure

Input Language for STRUCTURES

```
STRUCTURES
STRUCTURES  cid  atom1  atom2  bond / [atom1]  atom2  bond / ...
method-name  cid  groupno  noccur / groupno  noccur / ...
```

Input Language Description for STRUCTURES

STRUCTURES

Use when you choose the generalized method of defining molecular structure.

cid ..... Component ID

atom1, atom2 ..... Identifiers for a pair of atoms in the structure. An identifier is formed by the type of atom and the number assigned to it. For example, if the fifth atom in the structure is nitrogen, its identifier is N5. When *atom1* is the same as *atom2* of the previous pair, you can omit *atom1.* The atom types are:

C	Carbon
O	Oxygen
N	Nitrogen
S	Sulfur
B	Boron
SI	Silicon
F	Fluorine

CL	Chlorine
BR	Bromine
I	Iodine
AL	Aluminum
AS	Arsenic
BI	Bismuth
CD	Cadmium
GA	Germanium
GE	Gallium
HG	Mercury
P	Phosphorus
PB	Lead
SB	Antimony
SN	Tin
ZN	Zinc

bond ..... Type of bond that connects the atoms. To simplify the task of entering the structure of common ring compounds and saturated hydrocarbons, these special bond types have been defined:

S	Single bond
D	Double bond
T	Triple bond
B	Benzene ring
CYC5	Saturated 5-membered ring
CYC6	Saturated 6-membered ring
CYC7	Saturated 7-membered ring
SATC	Saturated hydrocarbon chain

When you use the special bond types, B, CYC5, CYC6, CYC7, and SATC, the atom numbers assigned to the members of the carbon ring or chain must be consecutive.

method-name Group contribution method from Table 8.4. These sentences are used to enter the group numbers and number of occurrences of each group when you choose the group method of defining molecular structure. Enter one *method-name* sentence for each group contribution method used. You can enter an unlimited number of pairs of *groupno* and *noccur*, except for the UNIFAC, UNIF-LL, UNIF-DMD, UNIF-LBY, AND UNIF-R4 methods, for which the limit is six.

cid..... Component ID

groupno ..... Group number. Obtain from *Aspen Plus Physical Property Data*, Tables 3.1 through 3.13.

noccur..... Number of occurrences of the group in the molecular structure of the component

Table 8.4 Group-Contribution Methods and Estimated Parameters

Method-Name	Property Parameters Estimated by This Method
AMBROSE	TC, PC, VC
BENSON	DHFORM, CPIG, DGFORM
BONDI	GMUFR, GMUFQ, GMUQR, GMUQQ
DUCROS	DHVLWT
GANI	TB, TC, PC, VC, DHFORM, DGFORM, DHVLWT
JOBACK	TB, TC, PC, VC, DHFORM, DGFORM, CPIG
LEBAS	RKTZRA
LI-MA	PLXANT, DHVLWT, SIGDIP
LYDERSEN	TC, PC, VC
MOSTAFA	DHSFRM, DGSFRM, CPSP01
OGATA-TSUCHIDA	TB
ORRICK-ERBAR	MULAND
PARACHOR	PARC
REICHENBERG	MUVDIP
RUZICKA	CPLDIP
UNIFAC	WILSON/2, NRTL/2, UNIQ/2, [WILSON/1], [NRTL/1], [UNIQ/1]
UNIF-LL	WILSON/2, NRTL/2, UNIQ/2, [WILSON/1], [NRTL/1], [UNIQ/1]
UNIF-DMD	WILSON/2, NRTL/2, UNIQ/2, [WILSON/1], [NRTL/1], [UNIQ/1]
UNIF-LBY	WILSON/2, NRTL/2, UNIQ/2, [WILSON/1], [NRTL/1], [UNIQ/1]
UNIF-R4	WILSON/2, NRTL/2, UNIQ/2, [WILSON/1], [NRTL/1], [UNIQ/1]

Entering Experimental Data

Input Language for PCES-PROP-DATA

```
PCES-PROP-DATA
propname   cid   temp   value / temp   value / ...
GAMINF   cid1   cid2      temp1   value1   temp2   value2 /
temp1   value1   temp2   value2 / ...
```

Input Language Description for PCES-PROP-DATA

propname

Name of the temperature-dependent property.

PL ..... Vapor pressure

VL ..... Liquid molar volume

DHVL..... Molar heat of vaporization

CPIG ..... Molar ideal gas heat capacity

CPL ..... Molar liquid heat capacity

CPS ..... Molar solid heat capacity

MUV ..... Vapor viscosity

MUL ..... Liquid viscosity

KV..... Vapor thermal conductivity

KL ..... Liquid thermal conductivity

SIGMA..... Surface tension

GAMINF

Use to enter infinite-dilution activity coefficients. If one infinite-dilution activity coefficient is not available, enter an asterisk (*) for both the temperature and value. In that case, Aspen Plus will use the UNIFAC method to estimate the missing infinite-dilution activity coefficient. If you enter several sets of data at different temperatures, Aspen Plus will determine both the first and second elements for the activity coefficient model (WILSON/1 and WILSON/2 parameters for the WILSON model).

cid, cid1, cid2..... Component IDs

temp ..... Temperature

value..... Property value

temp1 ..... Temperature for *value1*

value1..... Infinite-dilution activity coefficient of *cid1*

temp2 ..... Temperature for *value2*

value2..... Infinite-dilution activity coefficient of *cid2*

Note

1 Using PCES-PROP-DATA is similar to, but much easier than, using the Aspen Plus Data Regression System (DRS) to regress pure component temperature-dependent property data or infinite-dilution activity coefficient data.

PCES-PROP-DATA:

- Can be used in a simulation, TGS or ADA run
- Does not require you to identify the parameters to be regressed
- Does not require parameter initial guesses and limits
- Does not require you to specify data standard deviations

DRS provides unlimited flexibility. For example, with DRS you can:

- Mix VLE and pure component data
- Regress any parameter, such as an equation-of-state parameter
- Specify regression for only certain parameters in a correlation
- Provide standard deviations (weightings) for individual variables and data points

See Chapter 42 for a complete discussion of the Aspen Plus Data Regression System.

Report Options

Input Language for COMPARE

For comparing estimated versus experimental data:

```
COMPARE    cid  / ...
```

For comparing two components:

```
COMPARE    cid1    cid2  / ...
```

Input Language Description for COMPARE

cid, cid1, cid2 Component IDs

Defining User Property Parameters

This section describes the input language for defining user property parameters for user property models.

Input Language for USER-PROPS

```
USER-PROPS    paramname    [nset]    [paramtype]    [nel]  / ...
```

Input Language Description for USER-PROPS

Use the USER-PROPS paragraph to define additional parameters for your user property model.

paramname ..... Name of user-defined parameter to be used in user property model

nset ..... Maximum number of data sets allowed for this parameter

paramtype ..... Type of parameter:

1	Unary parameters for conventional components (Default)
2	Binary parameters for conventional components
3	Unary parameters for nonconventional components
4	Binary parameters for nonconventional components
5	Unary parameters for UNIFAC groups
6	Binary parameters for UNIFAC groups
8	Pair parameters for electrolytes

nel ..... Number of elements for the parameter (Default=1)

CAPE-OPEN Property Packages

This section describes the input language for referencing CAPE-OPEN property packages.

Input Language for CO-PACKAGE

```
CO-PACKAGE    pkgid
PARAM    [PACKAGENAME=value]    PROG-ID=value    BASE-METHOD=value
COMPONENTS    APNAME=value    CONAME=value    CASNUMBER=value / ...
```

Input Language Description for CO-PACKAGE

Use the CO-PACKAGE paragraph to reference a CAPE-OPEN property package for use in Aspen Plus.

pkgid ..... An ID identifying the package. You may use any number of CO-PACKAGE paragraphs, but the pkgid for each one must be unique.

PARAM Use to specify parameters identifying the CAPE-OPEN Property Package used.

PACKAGENAME ..... The name of the package, according to the CAPE-OPEN thermo system component. Optional.

PROG-ID ..... The prog-id of the CAPE-OPEN thermo system component to use.

BASE-METHOD ..... Base property method. This method is used as a fallback when the CAPE-OPEN method does not support a requested property.

COMPONENTS Use to a list of components and their mapping between Aspen Plus and the CAPE-OPEN package.

APNAME..... The Aspen Plus component ID for the component.

CONAME..... The name of the component in the CAPE-OPEN property package.

CASNUMBER..... Chemical Abstract Services registry number for the component.

9 Flowsheet and Hierarchy

This chapter describes the input language for using the FLOWSHEET and HIERARCHY paragraphs.

You can use the FLOWSHEET paragraph to:

- Specify the flowsheet connectivity.
- Order the outlet streams for certain unit operation blocks.

You can use the HIERARCHY paragraph to:

- Organize large flowsheets better.
- Use a hierarchical system of naming blocks and streams.

FLOWSHEET Paragraph

Input Language for FLOWSHEET

```
FLOWSHEET    [sectionid]
BLOCK    blockid    IN=sid-list    OUT=sid-list
HIERARCHY    hierid
CONNECT    conid    IN=sid    OUT=sid
```

Input Language Description for FLOWSHEET

sectionid ..... Flowsheet section ID. This ID is required only when a flowsheet is sectioned. You can section a flowsheet by including multiple FLOWSHEET paragraphs, one for each section. You can divide a flowsheet into sections to simplify the association of physical properties specifications with groups of blocks, or for clarity.

BLOCK

Use to specify the blocks in the flowsheet and the streams entering and leaving them.

blockid ..... Unit operation block ID

sid-list ..... List of stream IDs. Heat and work streams must be listed after the material streams.

HIERARCHY

Use to specify the Hierarchy blocks in the flowsheet. A Hierarchy block must be mentioned in a HIERARCHY sentence of a FLOWSHEET paragraph of the Hierarchy block's parent hierarchy level.

hierid ..... Hierarchy block ID

CONNECT

Use to specify stream connections into and out of Hierarchy blocks. One of the streams specified by IN and OUT must be at the current level of hierarchy, and the other must be in a Hierarchy block contained within this level of hierarchy.

conid..... Connect ID

sid..... Stream ID. The stream ID of the stream in the inner Hierarchy block must be specified hierarchically. For example: HB1.S1

HIERARCHY Paragraph

Input Language for HIERARCHY

```
HIERARCHY    hierid
FLOWSHEET    [sectionid]
[flowsheet paragraph input language]
BLOCK    blockid    blocktype
[block input language]

[other paragraphs]

ENDHIERARCHY    hierid
```

Input Language Description for HIERARCHY

HIERARCHY

Use to specify the beginning of input for a hierarchy block. All hierarchical input paragraphs until the corresponding ENDHIERARCHY statement are specified relative to this hierarchy block. Certain input paragraphs are not hierarchical; these are always treated as belonging to the top level of hierarchy, regardless of where they are located. See Table 9.1.

You can nest HIERARCHY blocks, but you must end inner ones before outer ones.

You can specify the contents of a HIERARCHY block in different sections of an input file, by specifying multiple HIERARCHY paragraphs at the same level of hierarchy with the same ID. See Example of Hierarchy Input Language.

The HIERARCHY and ENDHIERARCHY statements must begin in column one of an input line.

hierid ..... Hierarchy block ID. Can be up to 8 characters in length and cannot contain a period (.).

FLOWSHEET

Use to specify flowsheet connectivity within the Hierarchy block. Identical to the top-level FLOWSHEET paragraph described in this chapter, except for its placement in the hierarchy.

blockid ..... Unit operation block ID

BLOCK

Use to specify input for a block within the Hierarchy block. Identical to the BLOCK paragraph described in chapter 11, except for its placement in the hierarchy.

blockid ..... Unit operation block ID

blocktype ..... Unit operation block type

other paragraphs

Most other input language can also be used within a Hierarchy block. See Table 9.1 for a list of input language paragraphs which are treated hierarchically.

ENDHIERARCHY

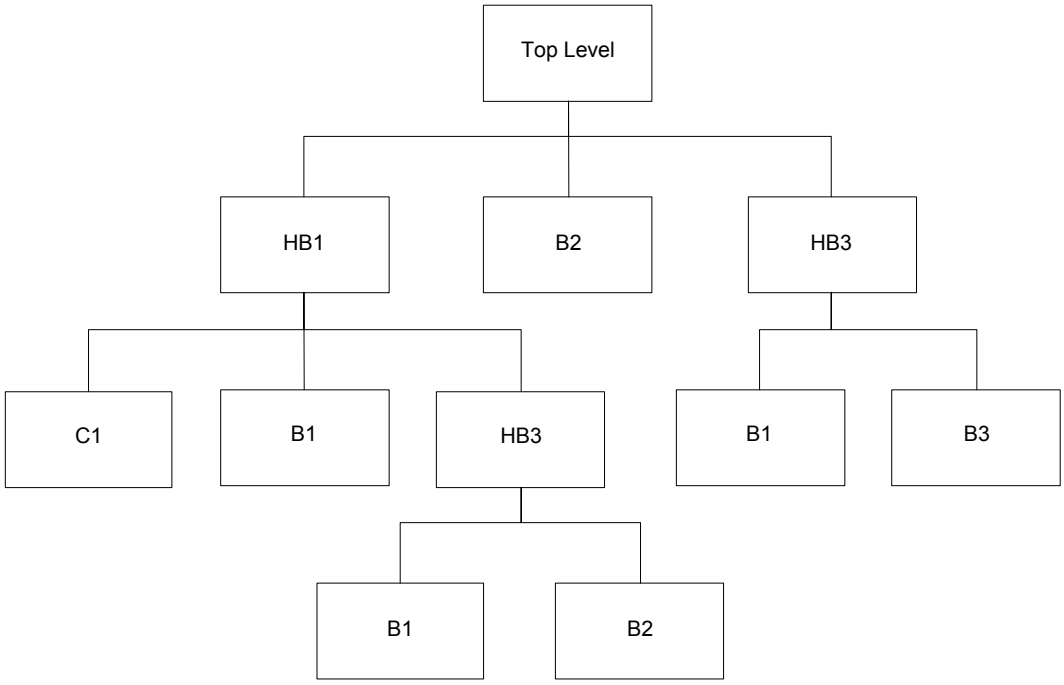
Use to specify the end of input for a hierarchy block.

hierid ..... Hierarchy block ID. Must match the hierid of the most recent unclosed HIERARCHY paragraph.

Hierarchical Input Language

A hierarchy block is a container for other Aspen Plus simulation objects (such as unit operation models, convergence blocks, and design specifications) and hierarchy blocks. The top level Aspen Plus flowsheet is a hierarchy block with no name, while other hierarchy blocks have names that uniquely identify these blocks.

In the hierarchy representation, normal and hierarchy blocks are organized into a tree. The top node of the tree is the hierarchy block that represents the whole flowsheet. Intermediate hierarchy block nodes represent sections of the flowsheet. Leaf nodes that have no children represent other Aspen Plus blocks. Consider, the following flowsheet hierarchy:



The four hierarchy blocks are Top Level (no name), HB1, HB1.HB3, and HB3. The normal Aspen Plus blocks are HB1.C1, HB1.B1, HB1.HB3.B1, HB1.HB3.B2, B2, HB3.B1, and HB3.B3. Note that these names are fully-qualified hierarchy object names. Also note that there are several B1 blocks that have different fully qualified names.

Example of Hierarchy Input Language

The following example illustrates the use of the input language for Hierarchy blocks.

The input not enclosed within HIERARCHY..ENDHIERARCHY belongs to the top level hierarchy.

```
IN-UNITS ...
FLOWSHEET
   BLOCK B2 IN=B2IN OUT=B2OUT
   HIERARCHY HB1
   HIERARCHY HB3
   CONNECT CNN1 IN=HB1.B1OUT OUT=B2IN

HIERARCHY HB1
```

The input here belongs to the HB1 hierarchy.

```
FLOWSHEET
   BLOCK B1 IN=B1IN OUT=B1OUT
   HIERARCHY HB3
BLOCK B1 FLASH2
   ...
```

The input here is for block HB1.B1

```
HIERARCHY HB3
```

The hierarchy context is now HB1.HB3

```
FLOWSHEET
BLOCK B1 MIXER
```

The input here is for block HB1.HB3.B1

```
BLOCK B2 FLASH2
```

The input here is for block HB1.HB3.B2

```
ENDHIERARCHY HB3
```

The hierarchy context is back to HB1

```
CALCULATOR C1
   DEFINE TEMP BLOCK-VAR BLOCK=HB3.B1 ...
```

Note that HB3.B1 specifies block HB1.HB3.B1 because the current hierarchy context is HB1

```
ENDHIERARCHY HB1
```

The hierarchy context is back to the top level. HIERARCHY and ENDHIERARCHY are nested. Always end the last pending hierarchy first

```
BLOCK B2 ...
```

The input here is for block B2

```
HIERARCHY HB1
```

The input here belongs to the HB1 hierarchy. It is OK to split input for hierarchy HB1 into several segments.

```
PROP-DATA DATA1 ...
```

Even though PROP-DATA is specified here, the data is still processed as if it is specified in the top level because PROP-DATA (like many other paragraph types) always belongs to the top level hierarchy.

```
HIERARCHY HB3
```

The hierarchy context is now HB1.HB3

```
FLOWSHEET
   ...
ENDHIERARCHY HB3
ENDHIERARCHY HB1
```

The hierarchy context is now top level hierarchy.

Hierarchical Input Paragraphs

Most Aspen Plus input language is hierarchical. In such input language, block and streams names are interpreted to be relative to the Hierarchy block containing it. For instance, within Hierarchy block HB1.HB2, a block that connects to stream S3 connects to the stream which is identified at the top level as HB1.HB2.S3. Some input language, such as COMPONENTS and CASE-STUDY, is not hierarchical, but instead is always treated as part of the top level, regardless where it appears in the input file. Table 9.1 lists the paragraphs which are hierarchical.

Table 9.1 Hierarchical Input Paragraphs

EO-ALIAS	DATA-SET	INIT-VAR-ATTR	RENAME
BALANCE	DEF-STREAMS	MEASUREMENT	SCRIPTMETHOD
BLOCK	DELETE	OBJECTIVE	SENSITIVITY
BLOCK-REPORT	DESIGN-SPEC	OPTIMIZATION	SEQUENCE
BYPRODUCT	EO-CONV-OPTI	PPTABLES	SOLVE
CALCULATOR	EO-OPTIONS	PRES-RELIEF	SPECGROUPS
CONNECTIONS	EO-PORT	PRODUCT	STREAM
CONSTRAINT	LOCALSCRIPT	PROFILE-DATA	STREAM-NAMES
CONVERGENCE	EOSENSITIVIT	PROPERTIES	STREAM-REPOR
COST-BLOCK	FLOWSHEET	PROP-TABLE	TRANSFER
CBLOCK-REPORT	FORTRAN	RAW-MATERIAL	UNIT-REPORT
UNIT	HIERARCHY	REGRESSION	WASTE

In hierarchical input language, HB1.HB3.B1 refers to the block B1 in Hierarchy block HB3 which is in Hierarchy block HB1 of the top level hierarchy. The same block is referenced as B1, HB3.B1, or HB1.HB3.B1 when mentioned in the input for HB1.HB3, HB1, and top level hierarchy respectively. Use proper names when accessing an object in lower level hierarchies in DEFINE, VARY, and SEQUENCE statements. To keep hierarchies self-contained, an object can only be accessed from its containing hierarchies. For example, HB1.HB3.B1 can be accessed from top level, HB1, and HB1.HB3 hierarchies but it cannot be accessed from the HB3 hierarchy. Due to this restriction it may be necessary to move some objects (such as CALCULATOR or DESIGN-SPEC) up the flowsheet hierarchy tree to access variables belong to other objects.

10 Streams

This chapter describes the input language used to:

- Specify conventional material streams.
- Define and modify general material streams (stream classes, substream classes, and substream attributes).
- Specify general material streams (consisting of any combination of MIXED, CISOLID, and NC substreams, and substream attributes).
- Specify heat and work streams.

Specifying Conventional Material Streams

Input Language for STREAM

```
STREAM    sid    keyword=value
```

Keywords:

TEMP PRES VFRAC basis-FLOW

Optional keywords:

NPHASE PHASE SOLVENT FREE-WATER MAXIT TOL FLASH-OPTION VOL-TREF CONC-TREF

```
basis–FLOW    cid    flow  / ...
basis–FRAC    cid    frac  / ...
basis-CONC    cid    conc  / ...
```

Input Language Description for STREAM

Use STREAM paragraphs to define the flow rates, composition, and thermodynamic condition of each process feed stream. Optionally, STREAM paragraphs can provide initial guesses for tear streams.

sid..... Stream ID

TEMP..... Temperature

PRES..... Pressure

VFRAC..... Molar vapor fraction

basis–FLOW..... Flow rate on a MOLE, MASS, STDVOL (standard-liquid volume) or VOLUME basis

NPHASE..... Number of phases:

NPHASE=1	One-phase calculation
NPHASE=2	Two-phase flash (Default)
NPHASE=3	Three-phase flash

PHASE..... Specifies the phase when NPHASE=1:

PHASE=V	Vapor (Default)
PHASE=L	Liquid
PHASE=S	Solid. Use for electrolytes system only.

SOLVENT..... Component ID of solvent. Use only when basis-CONC is specified.

FREE–WATER..... Use to override the free-water option established by the SIM-OPTIONS paragraph. (See Chapter 45.)

FREE–WATER=NO	Does not perform free-water calculations (Default)
FREE–WATER=YES	Performs free-water calculations

MAXIT..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

TOL ..... Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

FLASH–OPTION..... **FLASH-OPTION=NOFLASH** Suppresses the flash calculation (Default=performs flash calculations)

VOL-TREF..... Reference temperature for volume flows

CONC-TREF ..... Reference temperature for component concentrations

basis-FLOW Use to enter component flows on a MOLE, MASS, or STDVOL basis. If you specify component flows, the total flow is also specified. The component flows are then normalized.

cid..... Component ID (or an assay ID). (See Chapter 7.)

flow ..... Component MOLE, MASS, or STDVOL flow rate

basis-FRAC Use to enter component fractions on a MOLE, MASS, or STDVOL basis. You must also specify the total flow using the basis-FLOW tertiary keyword.

cid..... Component ID (or an assay ID). (See Chapter 7.)

frac ..... Component MOLE, MASS, or STDVOL fraction

basis-CONC Use to enter component concentration on a MOLE or MASS basis. You must also specify SOLVENT.

cid..... Component ID

conc..... Component concentration

Defining General Material Stream Classes

Input Language

```
DEF-STREAM-CLASS    sclass    ssid-list
DEF-SUBS    ssclass    ssid
DEF-SUBS-CLASS    ssclass
DEF    keyword=value
```

Keywords:

TYPE ATTR

```
DEF-SUBS-ATTR    psdid    PSD
INTERVALS    n
SIZE-LIMITS    limit1 / . . . / . . .    limit n+1
```

Input Language Description for DEF-STREAM-CLASS

Use the DEF-STREAM-CLASS paragraph to define new stream classes that are not built into the system. (See Table 10.1 for built-in substream classes.)

sclass..... Stream class. (See Table 10.2.)

ssid-list..... Substream ID list. MIXED must be the first substream ID.

Input Language Description for DEF-SUBS

Use the DEF-SUBS paragraph to assign a substream ID to a substream class.

ssclass ..... Substream class

ssid ..... Substream ID

Input Language Description for DEF-SUBS-CLASS

Use the DEF-SUBS-CLASS paragraph to create a new substream class (that is, to associate a substream type with a particle size distribution).

ssclass ..... Substream class

TYPE ..... Substream type (CISOLID or NC)

ATTR ..... Particle size distribution ID

Input Language Description for DEF-SUBS-ATTR

Use the DEF-SUBS-ATTR paragraph to specify size limits for the particle size distribution (PSD). This paragraph is used only with stream classes MIXCIPSD or MIXNCPSD.

psdid ..... Particle size distribution ID

INTERVALS Use to specify the number of discrete intervals in which to divide the particle size distribution

n ..... Number of intervals

SIZE-LIMITS Use to specify size limits for the discrete intervals. You must enter n+1 values, in ascending order, and separated by slashes.

limit ..... Size limit

Table 10.1 Built-In Substream Classes

Substream class	Substream ID	Substream type	Substream attribute ID
MIXED	MIXED	MIXED	—
CISOLID	CISOLID	CISOLID	—
NC	NC	NC	—
NCPSD	NCPSD	NC	PSD
CIPSD	CIPSD	CISOLID	PSD

Table 10.2 Built-In Material Stream Classes

Stream class	Number of substreams	Substream type(s)	Substream ID(s)
CONVEN	1	MIXED	MIXED
MIXCISLD	2	MIXED, CISOLID	MIXED, CISOLID
MIXNC	2	MIXED, NC	MIXED, NC
MIXCINC	3	MIXED, CISOLID, NC	MIXED, CISOLID, NC
MIXCIPSD	2	MIXED, CISOLID	MIXED, CIPSD
MIXNCPSD	2	MIXED, NC	MIXED, NCPSD
MCINCPSD	3	MIXED, CISOLID, NC	MIXED, CIPSD, NCPSD

Specifying General Material Streams

Input Language

```
DEF-STREAMS    sclass    { ALL | secid – list | sid – list }
STREAM    sid
SUBSTREAM    ssid    keyword=value
```

Keywords:

TEMP PRES VFRAC basis-FLOW

Optional keywords:

NPHASE PHASE SOLVENT FREE-WATER MAXIT TOL FLASH-OPTION

```
basis-FLOW    cid    flow / . . .
basis–FRAC    cid    frac  / . . .
basis-CONC    cid    conc  / . . .
COMP-ATTR    cid    cattrname    (value-list)
SUBS-ATTR    psdid    (value-list)
```

Input Language Description for DEF-STREAMS

Use the DEF-STREAMS paragraph to assign a stream class to a list of streams or to all the streams within flowsheet sections. (See Chapter 9.) There can be any number of DEF-STREAMS paragraphs. If you enter more than one DEF-STREAMS paragraph, the more general specifications should precede the more specific specifications. If you specify ALL, it must be in the first DEF-STREAMS paragraph for any streams in that section.

sclass ..... Stream class. (See Table 10.2.)

ALL ..... All streams in the flowsheet that are assigned to a specified stream class

secid-list ..... List of flowsheet section IDs

sid-list ..... List of stream IDs

Input Language Description for STREAM

Use the STREAM paragraph to specify inlet streams and initial guesses for tear streams.

sid ..... Stream ID

SUBSTREAM Use to enter state and flash specifications for substreams. For solid substreams, you must specify TEMP and PRES. The pressure of all substreams must be the same. For most applications the temperature of all substreams should be the same. RPLUG is the only Aspen Plus unit operation model that can treat a stream with substreams at different temperatures. Specify NPHASE and PHASE for the MIXED substream only. (See Table 10.3 for built-in substreams.)

ssid ..... Substream ID

TEMP ..... Temperature

PRES ..... Pressure

VFRAC ..... Molar vapor fraction (for MIXED substreams only)

basis-FLOW ..... Flow rate on a MOLE, MASS, or STDVOL basis

NPHASE ..... Number of phases in MIXED substream:

NPHASE=1	One-phase calculation
NPHASE=2	Two-phase flash (Default)
NPHASE=3	Three-phase flash

PHASE ..... Specifies the phase when NPHASE=1:

PHASE=V	Vapor
PHASE=L	Liquid
PHASE=S	Solid. Use for electrolytes system only.

SOLVENT ..... Component ID of solvent. Use only when basis-CONC is specified.

FREE–WATER ..... Use to override the free-water option established by the SIM-OPTIONS paragraph. (See Chapter 45.)

FREE–WATER=NO	Does not perform free-water calculations (Default)
FREE–WATER=YES	Performs free-water calculations

MAXIT ..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

TOL ..... Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

FLASH-OPTION ..... **FLASH-OPTION=NOFLASH** Suppresses the flash calculation (Default=performs flash calculations)

basis-FLOW

Use to enter component flow rates on a MOLE, MASS, or STDVOL basis. For substreams of type NC, only MASS basis is allowed. For substream of type CISOLID, only MOLE or MASS basis are allowed. If the basis-FLOW tertiary keyword is specified, the component flows are normalized.

cid ..... Component ID

flow ..... Component flow rate

basis-FRAC

Use to enter component fractions on a MOLE, MASS, or STDVOL basis. For substreams of type NC, only MASS basis is allowed. For substream of type CISOLID, only MOLE or MASS basis are allowed. You must specify the total flow using the basis-FLOW tertiary keyword.

cid ..... Component ID

frac ..... Component fraction

basis-CONC

Use to enter component concentration on a MOLE or MASS basis. For substreams of type NC, only MASS basis is allowed.

cid ..... Component ID

conc ..... Component concentration

COMP-ATTR

Use to enter component attributes for substreams of type NC. There should be one COMP-ATTR sentence for each component attribute specified.

cid ..... Component ID

cattrname ..... Component attribute name

value-list ..... List of attribute values. You should enter all values for the attribute, even if zero.

SUBS-ATTR

Use to enter particle size distribution values for substreams that have a particle size distribution attribute.

psdid..... Particle size distribution ID

value-list ..... List of substream weight fractions that lie within each particle size distribution interval

Table 10.3 Types of Substreams

This substream type	Handles
MIXED	Conventional components that participate in vapor-liquid-solid phase equilibrium
CISOLID (Conventional inert solids)	Conventional components that appear in the solid phase but do not participate in phase equilibrium
NC (Nonconventional)	Nonconventional components

Specifying Heat And Work Streams

Input Language

```
DEF-STREAMS   HEAT   sid-list
DEF-STREAMS   WORK   sid-list
STREAM   sid
INFO   HEAT   keyword=value
```

Keywords:

DUTY TEMP TEND

```
STREAM   sid
INFO   LOAD   TVEC=t1 t2 t3 t4   QVEC=q1 q2 q3 q4
STREAM   sid
INFO   WORK   POWER=power
```

Input Language Description

Use the DEF-STREAMS paragraph to define streams to be heat streams or work streams. Use the STREAM paragraph to enter the heat and work loads. Heat streams allow heat duties to pass from one process to another. Load streams are heat streams which include vectors describing the temperatures at which the heat was transferred. Work streams are similar to heat streams, except work streams carry information about power.

sid-list ..... List of all heat or work streams used in a simulation

sid..... Heat or work stream ID

DUTY..... Enthalpy flow rate

TEMP..... Starting temperature of a heat or load stream

TEND..... Ending temperature of a heat or load stream

t1, t2, t3, t4 ..... Temperature vector of a load stream

q1, q2, q3, q4..... Duty vector of a load stream

POWER ..... Power

Specifying Stream Names

Input Language for STREAM-NAMES

```
STREAM-NAMES
NAMES   sid   text
```

Input Language Description

Use the STREAM-NAMES paragraph to specify description for streams.

sid..... Stream id

text..... A string of any length enclosed in quotes. The description is printed under the Stream ID (up to 3 lines, each line is a maximum of 10 chars wide) in the STREAM-REPORT.

11 Block Data

This chapter describes the input language for general options of unit operation blocks. This chapter discusses:

- Block paragraphs.
- Heating and cooling curves.

It also includes information about properties, diagnostic levels, simulation options, and report options.

BLOCK Paragraphs

Input Language for BLOCK

BLOCK **blockid** **modelname**
DESCRIPTION **"a block description - up to 64 characters in quotes"**
PROPERTIES **opsetname** *keyword=value*

Optional keywords:

HENRY-COMPS **CHEMISTRY** **FREE-WATER** **SOLU-WATER** **TRUE-COMPS**

BLOCK-OPTIONS *keyword=value*

Optional keywords:

SIM-LEVEL **PROP-LEVEL** **STREAM-LEVEL** **TERM-LEVEL** **ENERGY-BAL** **RESTART** **FREE-WATER**

REPORT *reportopt-list*

Reportopts:

NOREPORT **NEWPAGE** **NOTOTBAL** **NOINPUT** **COMPBAL** **NORESULTS**

EO-OPTIONS **keyword=value**

Optional keywords:

COMPS **EO-FORM** **SPARSITY** **LIGHT-KEY**
HEAVY-KEY **DEP-COMPS** **DERIV-METHOD** **SOLVE-METHOD**
CHECK-FREE-W **NEG-COMP-CHK** **NEG-FLOW-CHK** **INLET-PHASE**

INIT-ATTR ***vname*** **keyword=value**

Optional keywords:

VALUE **LOWER** **UPPER** **STEP** **BOUND-TYPE** **SBWEIGHT**
PHYS-QTY **UOM** **SCALE**

EO-PORT **portid** **keyword=value**

Optional keywords:

VAR **VALUE** **TYPE** **COMPONENTS** **THRU** **PHASE** **PHYS-QTY**
UOM

SPEC-GROUP **specgroupid** **keyword=value**

Optional keywords:

ENABLED **COMMENT**

SPEC-CHANGE **specgroupid** **keyword=value**

Optional keywords:

VAR **SPEC**

EO-VAR keyword=value

Optional keywords:

SENTENCE VARIABLE ELEMENT ID1 ID2 ID3

EO-VEC keyword=value

Optional keywords:

SENTENCE VARIABLE

SCRIPTS keyword=value

Optional keywords:

METHOD TYPE LOCALSCRIPT GLOBALSCRIPT FILE

Input Language Description for BLOCK

You must enter one BLOCK paragraph for each unit operation block in the simulation. A simulation must contain at least one unit operation block.

blockid ..... Block ID

modelname ..... Unit operation model name. (See Table 11.1.)

DESCRIPTION A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the block report.

PROPERTIES Use to replace the flowsheet or section property specifications. Any option set name you enter here must also be named in the PROPERTIES paragraph. (See Chapter 8.)

BLOCK-OPTIONS Use to override the diagnostic message levels, established by the DIAGNOSTICS paragraph. (See Chapter 45.) It also overrides simulation options established by the SIM-OPTIONS paragraph. (See Chapter 45.) Table 11.1 lists the free-water and three-phase options available for each unit operation model.

REPORT Use to suppress the block report, or to replace the report options established in the BLOCK-REPORT paragraph. (See Chapter 46.)

EO-OPTIONS Use to specify equation-oriented options for the block.

COMPS ..... Component group for a list of components which can be active in this block.

EO-FORM ..... Equation-oriented formulation.

EO-FORM=STANDARD	Standard formulation. Compositions in terms of mole fractions. Stream variables named using Aspen Plus stream names.(Default)
EO-FORM=EOPML	For RT-Opt 10.0 / DMO compatibility. Compositions in terms of mole fractions. Stream variables named using PML convention.
EO-FORM=MOLEFRAC	For RT-Opt 10.0 compatibility. Compositions in terms of molar fractions. Stream variables named using PML convention. Some reduced functionality.
EO-FORM-MOLEFLOW	For RT-Opt 3.0 compatibility. Compositions in terms of molar flows. Stream variables named using Aspen Plus stream names.

SPARSITY ..... Used to set the dependence of thermodynamic properties on state variables and compositions while evaluating derivatives.

SPARSITY=FULL	Temperature, pressure and composition dependence.

SPARSITY=COMP-INDEP	Temperature and pressure dependence.
SPARSITY=WATER-SOLU	Temperature, pressure and composition dependence for water, temperature and pressure dependence for all other components.

LIGHT-KEY ..... Component ID of the lightest distributing component.

HEAVY-KEY ..... Component ID of the heaviest distributing component.

DEP-COMPS ..... Component group of components for which fugacities are composition dependent. Pure component fugacities are used for all other components.

DERIV-METHOD ..... Preferred derivatives method, Analytic or Numeric. Update methods should not be used for Degree of Freedom run modes (Optimization or Reconciliation).

DERIV-METHOD = ANALYTICAL	Model derivatives (Jacobian) are determined from coded analytic expressions. Generally the preferred method. (Default)
DERIV-METHOD = NUMERICAL	Alternate method for calculating Jacobian. Useful when there is concern that analytic derivatives are causing convergence difficulties. Usually slower than analytic derivatives, more subject to precision issues.
DERIV-METHOD = UPDATE-ANALY	Use Schubert method for updating Jacobian. Base Jacobian via analytic derivatives. Use when Jacobian calculation is rate limiting step. May result in more iterations and be less robust than calculated derivatives.
DERIV-METHOD = UPDATE-NUMER	Use Schubert method for updating Jacobian. Base Jacobian via numerical derivatives. Use when Jacobian calculation is rate limiting step. May result in more iterations and be less robust than calculated derivatives.

SOLVE-METHOD ..... EO solution method. Specifies if open, closed, or neither method should be used with desired action and message level on failure.

SOLVE-METHOD = OPEN-PERT-IN	Open solution method; on failure use Perturbation with information messages. (Default)
SOLVE-METHOD = OPEN-PERT-WA	Open solution method; on failure use Perturbation with warning messages.
SOLVE-METHOD = OPEN-NOPERT	Open solution method; on failure stop with error messages.
SOLVE-METHOD= PERTURBATION	Closed solution method; use Perturbation layer around closed model.
SOLVE-METHOD= DO-NOT-CREAT	Ignore during EO solution.

CHECK-FREE-W ..... Check if only water appears in a stream when Free-Water=Yes. If so, turn off Free-Water in VLE calculations, and do not consider the existence of any other components.

CHECK-FREE-W = YES	Check for presence of only water. (Default)
CHECK-FREE-W = NO	Do not check for presence of only water.

NEG-COMP-CHK ..... Negative composition check/Value used to check for negative mole fractions and issue warnings during the report phase. (Default=-$1x10^{-8}$)

NEG-FLOW-CHK ..... Negative flow check/Value used to check for negative mole flow and issue warnings during the report phase. (Default=0.0)

INLET-PHASE ..... Phase for the Material port. If unspecified, the phase will be obtained from the upstream conditions.

INLET-PHASE = V	Vapor only.
INLET-PHASE = L	Liquid only
INLET-PHASE = MIXED	Vapor-Liquid or Vapor-Liquid-FreeWater, depending on the block's free-water option.

INIT-ATTR Use to specify the attributes of open variables.

vname..... Name of the variable. (Required)

VALUE..... Current value of the variable.

LOWER..... Lower bound.

UPPER..... Upper bound.

STEP ..... Step bound.

BOUND-TYPE ..... Bound type.

BOUND-TYPE = HARD	Do not violate the upper and/or lower bounds when solving a non-square (optimization or data regression) problem.
BOUND-TYPE = RELAXED	Relax upper and/or lower bound. If the initial value is outside the bound, set the bound to the initial value.
BOUND-TYPE = SOFT	Same as relaxed but add a penalty term to the objective to try to drive the value back to the bound.

SBWEIGHT..... Soft bound weight.

PHYS-QTY..... The physical quantity that the variable represents, for example, mole flow, temperature, or pressure. These types correspond to the standard Aspen Plus types.

UOM..... Units of measure (standard Aspen Plus units), based on the physical type of the variable. Internally, all values are stored in SI units.

SCALE ..... Scale factor used by the solver.

EO-PORT Use this sentence to define the variables that make up a port. A port is an arbitrary collection of variables. Ports can make connecting groups of variables easier.

portid..... Name of the port. (Required)

VAR..... Open variable name.

VALUE..... Initial value.

TYPE ..... Type of port.

TYPE = MOLE-FLOW	Material stream (flow basis).
TYPE = MOLE-FRAC	Material stream (fraction basis).
TYPE = HEAT	Heat stream.
TYPE = WORK	Work stream.
TYPE = GENERIC	Generic collection.

COMPONENTS ..... Comp-Group ID. Correction for the component list if the global component list is not being used.

THRU ..... Specifies whether to include all variables from VAR in this EO-PORT sentence through VAR in the next EO-PORT sentence.

THRU = YES	Include all variables.
THRU = NO	Do not include all variables. (Default)

PHASE ..... Phase for the material port. If unspecified, the phase will be obtained from the upstream conditions.

PHASE = V	Vapor only.
PHASE = L	Liquid only.
PHASE = VL	Vapor and Liquid.
PHASE = VLW	Vapor, Liquid, and Free-Water.

PHYS-QTY ..... The physical quantity that the variable represents, for example, mole flow, temperature, or pressure. These types correspond to the standard Aspen Plus types.

UOM ..... Units of measure (standard Aspen Plus units), based on the physical type of the variable. Internally, all values are stored in SI units.

SPEC-GROUP Use this sentence to override default variable specifications. Each spec group must not change the net specification of the problem.

specgroupid ..... Spec group name. (Required)

ENABLED ..... Whether the spec group is enabled or disabled.

ENABLED = YES	Spec group is enabled. (Default)
ENABLED = NO	Spec group is disabled.

COMMENT ..... Optional comment associated with the spec group.

SPEC-CHANGE Use the sentence to add a variable to a spec group.

specgroupid ..... Spec group name. (Required)

VAR Open variable name.

SPEC ..... Change applied by the user to change the initial specification.

SPEC = CALC	Calculated.
SPEC = CONST	Constant.
SPEC = INDEP	Independent
SPEC = MEAS	Measured.
SPEC = PARAM	Parameterized
SPEC = OPTIM	Optimized.
SPEC = RECON	Reconciled.

EO-VAR Use the sentence to specify scalar sequential-modular variables to be exposed as equation-oriented variables when the block is being run via the perturbation layer.

SENTENCE ..... Sentence name.

VARIABLE ..... Closed variable name.

ELEMENT ..... Element number for array variable.

ID1 ..... First ID.

ID2 ..... Second ID.

ID3 ..... Third ID.

EO-VEC Use the sentence to specify vector sequential-modular variables to be exposed as equation-oriented variables when the block is being run via the perturbation layer.

SENTENCE ..... Sentence name.

VARIABLE ..... Closed variable name.

SCRIPTS Use this sentence to specify scripts for a block.

METHOD ..... Script method. Blocks support default script methods of SETUP and INIT. User may define other methods. (Required)

TYPE ..... Type of script (Required)

TYPE = LOCALSCRIPT	Local Script
TYPE = GLOBALSCRIPT	Global Script
TYPE = FILE	File

LOCALSCRIPT ..... ID of a LOCAL SCRIPT paragraph

GLOBALSCRIPT ..... ID of a GLOBAL SCRIPT paragraph

FILE ..... Name of a file

Table 11.1 Unit Operation Models

Model	Description	Heating and cooling curves	Free-water calculations	Water decanter streams	Rigorous three-phase calculations	Chapter
MIXER	Stream mixer	No	Yes	Yes	Yes	12
FSPLIT	Stream splitter	No	Yes	No	Yes	12
SSPLIT	Substream splitter	No	Yes	No	Yes	12
SEP	Component separator	No	Yes	No	Yes	12
SEP2	Two outlet component separator	No	Yes	No	Yes	12
HEATER	Heater/cooler	Yes	Yes	Yes	Yes	13
FLASH2	Two outlet flash	Yes	Yes	Yes	Yes	13
FLASH3	Three outlet flash	Yes	No	No	Yes	13
DECANTER	Liquid-liquid decanter	Yes	Yes	No	Yes	13
HEATX	Two stream heat exchanger	Yes	Yes	Yes	Yes	13
MHEATX	Multistream heat exchanger	Yes	Yes	Yes	Yes	13
HXFLUX	Heat transfer calculation	No	No	No	No	13
HETRAN	Shell and tube heat exchanger	No	Yes	Yes	Yes	13
AEROTRAN	Air-cooled heat exchanger	No	Yes	Yes	Yes	13
HTRIXIST	Shell and tube heat exchanger	No	Yes	Yes	Yes	13
DSTWU	Shortcut distillation design	No	Yes†	Yes	No††	14
DISTL	Shortcut distillation rating	No	Yes†	Yes	No††	14
SCFRAC	Shortcut distillation for petroleum	No	Yes†	No	No††	14
RADFRAC	Rigorous distillation	Yes	Yes	Yes	Yes	15
MULTIFRAC	Rigorous distillation for complex columns	Yes	Yes	Yes	No††	15
PETROFRAC	Rigorous distillation for petroleum	Yes	Yes	Yes	No	15
EXTRACT	Rigorous liquid-liquid extractor	No	No	No	—	18
RSTOIC	Stoichiometric reactor	No	Yes	Yes	Yes	19
RYIELD	Yield reactor	No	Yes	Yes	Yes	19
REQUIL	Equilibrium reactor	No	No	No	No	19
RGIBBS	Equilibrium reactor	No	No	No	Yes♦	19
RCSTR	Continuous stirred tank reactor	No	Yes	No	Yes	19
RPLUG	Plug flow reactor	No	Yes	No	Yes	19
RBATCH	Batch reactor	No	Yes	No	Yes	19

† Rigorous liquid-liquid equilibrium calculations.

†† Condenser only.

♦ RGIBBS handles any number of phases rigorously.

continued

Table 11.1 Unit Operation Models (continued)

Model	Description	Heating and cooling curves	Free-water calculations	Water decanter streams	Rigorous three-phase calculations	Chapter
PUMP	Pump/hydraulic turbine	No	Yes	Yes	Yes	20
COMPR	Compressor/turbine	No	Yes	Yes	Yes	20
MCOMPR	Multistage compressor/turbine	Yes	Yes	Yes	Yes	20
PIPELINE	Pipe pressure drop (multiple segments)	No	Yes	No	Yes	21
PIPE	Pipe pressure drop (single segment)	No	Yes	No	Yes	21
VALVE	Valve	No	Yes	No	Yes	21
CRYSTALLIZER	Mixed-suspension, mixed-product removal crystallizer	No	No	No	No	22
CRUSHER	Solids crusher	No	Yes	No	No	23
SCREEN	Solids separator	No	Yes	No	No	23
FABFL	Fabric filter	No	Yes	No	No	24
CYCLONE	Cyclone separator	No	Yes	No	No	24
VSCRUB	Venturi scrubber	No	Yes	No	No	24
ESP	Electrostatic precipitator	No	Yes	No	No	24
HYCYC	Hydrocyclone	No	Yes	No	No	25
CFUGE	Centrifuge filter	No	Yes	No	No	25
FILTER	Rotary vacuum filter	No	Yes	No	No	25
SWASH	Single-stage solids washer	No	Yes	No	No	26
CCD	Counter-current decanter	No	Yes	No	No	26
MULT	Stream multiplier	No	—	—	—	27
DUPL	Stream duplicator	No	—	—	—	27
CLCHNG	Stream class changer	No	—	—	—	27
SELECTOR	Stream selector	No	—	—	—	27
QTVEC	Load stream manipulator	No	—	—	—	27
ANALYZER	Stream calculator	No	—	—	—	27
USER	User-supplied unit operation model	No	Yes	No	Yes	28
USER2	User-supplied unit operation model	No	Yes	No	Yes	28
USER3	User-supplied unit operation model	No	Yes	No	Yes	28

Heating and Cooling Curve

Input Language for HCURVE

HCURVE **curveno** *keyword=value*

Optional keywords:

INDEP-VAR LIST NPOINT INCR HEADING PROPERTIES PRES-PROFILE PDROP PRINT-PLOT HIGH-PRECISION LINES X-SCALE Y-SCALE WIDE GRID INTERPOLATE

Input Language Description for HCURVE

HCURVE

Use to enter all specifications for a single heating or cooling curve table or plot. Aspen Plus generates one table for each HCURVE sentence you enter. Multiple tables are generated by entering multiple HCURVE sentences, each with a different curve number. You can use only one of the keywords (LIST, NPOINT, or INCR) in an HCURVE sentence. The default is NPOINT=10. See Table 11.1 for more information about unit operation models.

curveno..... Curve number

INDEP-VAR ..... Independent variable used to generate intermediate points:

INDEP-VAR=TEMP	Temperature
INDEP-VAR=VFRAC	Vapor fraction
INDEP-VAR=DUTY	Heat duty (Default)

LIST ..... List of independent variable point values. This list can extend beyond the inlet and outlet values.

NPOINT ..... Number of intermediate point values (Default=10)

INCR ..... Increment size for the independent variable between intermediate points

HEADING ..... String of up to 60 characters in quotes

PROPERTIES ..... List of property set IDs. (See Chapter 41.)

PRES-PROFILE ..... Pressure profile option (Default=CONSTANT)

If the PRES-PROFILE is	The first point is	The last point is
CONSTANT	Outlet Pressure	Outlet Pressure
LINEAR	Inlet Pressure – PDROP	Outlet Pressure
LINEAR2	Inlet Pressure	Inlet Pressure – PDROP
LINEAR3	Outlet Pressure + PDROP	Outlet Pressure
OUTLET	Outlet Pressure	Outlet Pressure
INLET	Inlet Pressure	Inlet Pressure
MID-POINT	(Outlet + Inlet)/2	(Outlet + Inlet)/2
CONSTANT2	Inlet Pressure – PDROP	Inlet Pressure – PDROP
CONSTANT3	Inlet Pressure + PDROP	Inlet Pressure + PDROP

PDROP ..... Pressure drop used in calculating the pressure profile (Default=0)

PRINT-PLOT	**PRINT-PLOT=YES**	Produces print-plots of all tabular values (except pressure) versus the independent variable
	PRINT-PLOT=NO	Does not produce print-plots (Default)
HIGH-PRECISION	**HIGH-PRECISION=YES**	Prints seven significant digits in tables
	HIGH-PRECISION=NO	Prints five significant digits in tables (Default)

LINES ..... Number of rows of values to print in tables before printing a grid line. If LINES=0, no grid lines are printed. The number must be between 0 and 35. (Default=5)

X-SCALE	**X-SCALE=STANDARD**	Uses linear scale on horizontal axis of plots (Default)
	X-SCALE=INVERSE	Uses inverse scale on horizontal axis of plots
Y-SCALE	**Y-SCALE=STANDARD**	Uses linear scale on vertical axis of plots (Default)
	Y-SCALE=INVERSE	Uses inverse scale on vertical axis of plots
	Y-SCALE=LOG	Uses logarithmic scale on vertical axis of plots

WIDE, GRID, INTERPOLATE ..... Plot options. Use to override defaults established by the PLOT-OPTIONS paragraph. (See Chapter 46.)

12 Mixers and Splitters

This chapter describes the input language for models that mix and split streams. The models are:

Model	Description	Purpose	Use
MIXER	Stream mixer	Combine streams into one stream	Mixing tees; stream mixing operations; adding heat streams; adding work streams
FSPLIT	Stream splitter	Split stream flows	Stream splitters; bleed valves
SSPLIT	Substream splitter	Divide inlet streams into component substreams	Stream splitters; perfect fluid-solid separators
SEP	Component separator	Separate inlet stream components into outlet streams	Component separation operations (such as distillation and absorption), when the details of the separation are unknown or unimportant
SEP2	Two-outlet component separation	Separate inlet stream components into two outlet streams	Component separation operations (such as distillation and absorption), when the details of the separation are unknown or unimportant

MIXER: Stream Mixer

Input Language for MIXER

```
BLOCK    blockid    MIXER
PARAM    keyword=value
```

Optional keywords:

PRES NPHASE PHASE MAXIT TOL T-EST

Input Language Description for MIXER

PARAM

Use to specify the outlet conditions. If you do not specify the outlet pressure, it defaults to the minimum pressure of the inlet streams.

PRES	**PRES > 0**	Pressure
	PRES ≤ 0	Pressure drop (Default=0)
NPHASE	Number of phases in MIXED substream:	
	NPHASE = 1	One-phase calculation
	NPHASE = 2	Two-phase flash (Default)
	NPHASE = 3	Three-phase flash
PHASE	Specifies phase when NPHASE=1:	
	PHASE = V	Vapor (Default)
	PHASE = L	Liquid
	PHASE = S	Solid. Use for electrolytes system only.
MAXIT	Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	
TOL	Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	
T-EST	Temperature estimate. Use to aid convergence.	

Accessing Variables in MIXER

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following table lists variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables
PARAM	PRES, MAXIT, TOL, T-EST

FSPLIT: Stream Splitter

Input Language for FSPLIT

```
BLOCK    blockid    FSPLIT
PARAM    keyword=value
```

Optional keywords:

PRES NPHASE PHASE MAXIT TOL

```
FRAC    sid    frac  /  ...
basis-FLOW    sid    flow    [keyno]  /  ...
VOL-FLOW    sid    flow  /  ...
basis-LIMIT    sid    flow  /  ...
VOL-LIMIT    sid    flow  /  ...
basis-C-LIM    sid    flow  /  ...
VOL-C-LIM    sid    flow  /  ...
R-FRAC    sid    frac  /  ...
STREAM-ORDER    sid    order    /  ...
DEF-KEY    KEYNO=keyno    SUBSTREAM=ssid    COMPS=cid-list  /  &
SUBSTREAM=ssid    COMPS=cid-list  /  ...
```

Input Language Description for FSPLIT

PARAM Use to specify outlet conditions. If you do not specify the pressure, it defaults to the minimum pressure of the inlet streams.

PRES	**PRES > 0**	Pressure
	PRES ≤ 0	Pressure drop (Default=0)
NPHASE	Number of phases in MIXED substream:	
	NPHASE = 1	One-phase calculation
	NPHASE = 2	Two-phase flash (Default)
	NPHASE = 3	Three-phase flash
PHASE.....	Specifies the phase when NPHASE=1:	
	PHASE = V	Vapor (Default)
	PHASE = L	Liquid
	PHASE=S	Solid. Use for electrolytes system only.
MAXIT.....	Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	
TOL.....	Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	

FRAC Use to specify the fraction of the inlet stream going to an outlet stream.

sid.....	Outlet stream ID
frac.....	Split fraction

basis-FLOW Use to specify the flow rate on a MOLE, MASS, or STDVOL basis of an outlet stream. If a key is given, use to specify the flow rate of a subset of components in an outlet stream. You cannot use STDVOL basis if any solid substreams are present. You can use only MASS basis if a substream type NC is present.

sid.....	Outlet stream ID
flow	Flow rate

keyno..... Key number

VOL-FLOW Use to specify the actual volumetric flow rate of an outlet stream.

sid..... Outlet stream ID

flow ..... Actual volumetric flow rate

basis-LIMIT Use to specify the limit flow rate on a MOLE, MASS, or STDVOL basis of an outlet stream. You cannot use STDVOL basis if any solid substreams are present. You can use only MASS basis if a substream of type NC is present.

sid..... Outlet stream ID

flow ..... Limit flow rate

VOL-LIMIT Use to specify the actual volumetric limit flow rate of an outlet stream.

sid..... Outlet stream ID

flow ..... Actual volumetric limit flow rate

basis-C-LIM Use to specify the cumulative limit flow rate on a MOLE, MASS, or STDVOL basis of an outlet stream. You cannot use STDVOL basis if any solid substreams are present. You can use only MASS basis if a substream type NC is present.

sid..... Outlet stream ID

flow ..... Cumulative limit flow rate

VOL-C-LIM Use to specify the actual volumetric cumulative limit flow rate of an outlet stream.

sid..... Outlet stream ID

flow ..... Actual volumetric cumulative limit flow rate

R-FRAC Similar to FRAC, except use to specify the fraction of the residue going into an outlet stream. In this case, the residue is the flow of the inlet remaining after all other specifications (FRAC, basis-FLOW, VOL-FLOW, basis-LIMIT, VOL-LIMIT, basis-C-LIM, and VOL-C-LIM) are satisfied.

sid..... Outlet stream ID

frac..... Split fraction

STREAM-ORDER Use to specify order of flow split calculation for outlet streams.

sid..... Outlet stream ID

order..... Order of flow split calculation for outlet streams. Use numbers 1 to the number of outlet streams to specify the order.

DEF-KEY Use to define the keys by associating a component or a group of components with a key number. One DEF-KEY statement is required for each key defined.

keyno..... Key number

ssid..... Substream ID (Default=MIXED)

cid-list ..... List of component IDs

Accessing Variables in FSPLIT

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following table lists variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1
PARAM	PRES, MAXIT, TOL	—
FRAC	FRAC	sid
basis-FLOW	FLOW	sid
VOL-FLOW	FLOW	sid
basis-LIMIT	FLOW	sid
VOL-LIMIT	FLOW	sid
basis-C-LIM	FLOW	sid
VOL-C-LIM	FLOW	sid
R-FRAC	FRAC	sid

SSPLIT: Substream Splitter

Input Language for SSPLIT

```
BLOCK    blockid    SSPLIT
PARAM    keyword=value
```

Optional keywords:

PRES NPHASE PHASE MAXIT TOL

```
FRAC    ssid    sid    frac  /  sid    frac  /  ...
basis-FLOW    ssid    sid    flow    keyno  /  sid    flow    keyno  /  ...
DEF-KEY    KEYNO=keyno    COMPS=cid-list
```

Input Language Description for SSPLIT

PARAM

Use to specify outlet conditions. If you do not specify the pressure, it defaults to the minimum pressure of the inlet streams.

PRES	**PRES > 0**	Pressure
	PRES ≤ 0	Pressure drop (Default=0)
NPHASE	Number of phases in MIXED substream:	
	NPHASE = 1	One-phase calculation
	NPHASE = 2	Two-phase flash (Default)
	NPHASE = 3	Three-phase flash
PHASE.....	Specifies the phase when NPHASE=1:	
	PHASE = V	Vapor (Default)
	PHASE = L	Liquid
	PHASE = S	Solid. Use for electrolytes system only.

MAXIT ..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

TOL ..... Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

FRAC

Use to specify the fraction of the inlet stream going to an outlet stream.

ssid ..... Substream ID

sid ..... Outlet stream ID

frac ..... Split fraction

basis-FLOW

Use to specify the flow rate on a MOLE, MASS, or STDVOL basis of an outlet stream. If a key is given, use to specify flow rate of a subset of components in an outlet stream. You cannot use STDVOL basis if any solid substreams are present. You can use only MASS basis if a substream type NC is present.

ssid ..... Substream ID

sid ..... Outlet stream ID

flow ..... Flow rate

keyno ..... Key number (allowed only when basis-FLOW is in MOLE or MASS basis)

DEF-KEY

Use to define the keys by associating a component or a group of components with a key number. One DEF-KEY statement is required for each key defined.

keyno ..... Key number

cid-list ..... List of component IDs

Accessing Variables in SSPLIT

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following table lists variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	ID2
PARAM	PRES, MAXIT, TOL	—	—
FRAC	FRAC	ssid	sid
basis-FLOW	FLOW	ssid	sid

SEP: Component Separator

Input Language for SEP

```
BLOCK    blockid    SEP
PARAM    keyword=value
```

Optional keywords:

PRES NPHASE PHASE MAXIT TOL

```
FRAC    SUBSTREAM=ssid    STREAM=sid    COMPS=cid-list    FRACS=frac-list
basis-FLOW    SUBSTREAM=ssid    STREAM=sid    COMPS=cid-list    FLOWS=flow-
list
FLASH-SPECS    sid    keyword=value
```

Keywords:

TEMP PRES DELT VFRAC

Optional keywords:

NPHASE PHASE FREE-WATER MAXIT TOL KODE T-EST P-EST

```
UTILITY    UTILITY-ID=utilityid
```

Input Language Description for SEP

PARAM

Use to specify block pressure and inlet flash options. If you do not specify the pressure, it defaults to the minimum pressure of the inlet streams. If an outlet stream pressure is different from the block pressure, use the FLASH-SPECS sentence to specify the outlet pressure.

PRES	**PRES > 0**	Pressure
	PRES ≤ 0	Pressure drop (Default=0)
NPHASE	Number of phases in MIXED substream:	
	NPHASE = 1	One-phase calculation
	NPHASE = 2	Two-phase flash (Default)
	NPHASE = 3	Three-phase flash
PHASE	Specifies the phase when NPHASE=1:	
	PHASE = V	Vapor (Default)
	PHASE = L	Liquid
	PHASE = S	Solid. Use for electrolytes system only.
MAXIT	Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	
TOL	Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	

FRAC

Use to specify the fraction of components in the inlet going to an outlet stream.

sid	Outlet stream ID
ssid	Substream ID (Default=MIXED)
cid-list	List of component IDs
frac-list	List of split fractions corresponding to *cid-list*

basis-FLOW Use to specify the flow rate of components in an outlet stream on a MOLE, MASS, or STDVOL basis. For substreams of type NC, only MASS basis is allowed. For substream of type CISOLID, only MOLE and MASS basis are allowed.

sid ..... Outlet stream ID

ssid ..... Substream ID (Default=MIXED)

cid-list ..... List of component IDs

flow-list ..... List of component flow rates corresponding to *cid-list*

FLASH-SPECS Use to specify the conditions of the outlet streams. The default is a TP flash using the block pressure and temperature.

sid ..... Stream ID

TEMP ..... Temperature

PRES ..... Pressure

DELT ..... Temperature difference

VFRAC ..... Molar vapor fraction. Enter 0.0 for bubble point, 1.0 for dew point. For subcooled liquid or superheated vapor, use TEMP and PRES specifications.

NPHASE ..... Number of phases in MIXED substream:

NPHASE = 1	One-phase calculation
NPHASE = 2	Two-phase flash (Default)
NPHASE = 3	Three-phase flash

PHASE ..... Specifies the phase when NPHASE=1:

PHASE = V	Vapor (Default)
PHASE = L	Liquid
PHASE = S	Solid. Use for electrolytes system only.

FREE-WATER ..... Use to override the free-water option established by the SIM-OPTIONS paragraph. (See Chapter 45.) Or use to override the BLOCK-OPTIONS sentence of the block paragraph. (See Chapter 11.)

FREE-WATER = NO	Does not perform free-water calculations.
FREE-WATER = YES	Performs free-water calculations.

MAXIT ..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

TOL ..... Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

KODE ..... **KODE=NOFLASH** Suppresses flash calculations (Default=performs flash calculations)

T-EST ..... Temperature estimate for outlet stream. Use to aid convergence when PRES and VFRAC are specified.

P-EST ..... Pressure estimate for outlet stream. Use to aid convergence when TEMP and VFRAC are specified.

UTILITY Use to specify an optional utility to provide heating or cooling duty.

UTILITY-ID ..... Utility ID.

Accessing Variables in SEP

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following table lists variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	ID2	Element
PARAM	PRES, MAXIT, TOL	—	—	—
FRAC	FRACS	ssid	sid	†
basis-FLOW	FLOWS	ssid	sid	†
FLASH-SPECS	TEMP, PRES, DELT, VFRAC, T-EST, P-EST, MAXIT, TOL	sid	—	—

† Component number of a component in the COMPS cid-list.

Block Results

Description	Sentence	Variable
Heat duty	RESULTS	QCALC

SEP2: Two-Outlet Component Separator

Input Language for SEP2

BLOCK **blockid** **SEP2**
PARAM *keyword=value*

Optional keywords:

PRES **NPHASE** **PHASE** **MAXIT** **TOL**

STREAM-FRAC **ssid** **sid** **frac / ...**
STREAM-MOLE-FLOW **ssid** **sid** **flow / ...**
STREAM-MASS-FLOW **ssid** **sid** **flow / ...**
STREAM-STDVOL-FLOW **[MIXED]** **sid** **flow / ...**
FRAC **[SUBSTREAM=ssid]** **STREAM=sid** **COMPS=cid-list** **FRACS=frac-list**
basis-FLOW **[SUBSTREAM=ssid]** **STREAM=sid** **COMPS=cid-list** **FLOWS=flow-list**
MOLE-FRAC **[SUBSTREAM=ssid]** **STREAM=sid** **COMPS=cid-list** **FRACS=frac-list**
MASS-FRAC **[SUBSTREAM=ssid]** **STREAM=sid** **COMPS=cid-list** **FRACS=frac-list**
FLASH-SPECS **sid** *keyword=value*

Keywords:

TEMP **PRES** **DELT** **VFRAC**

Optional keywords:

NPHASE **PHASE** **FREE-WATER** **MAXIT** **TOL** **KODE** **T-EST** **P-EST**

UTILITY **UTILITY-ID=***utilityid*

Input Language Description for SEP2

PARAM Use to specify the block pressure and inlet flash options. If you do not specify the pressure, it defaults to the minimum pressure of the inlet streams. If an outlet stream pressure is different from the block pressure, use the FLASH-SPECS sentence to specify the outlet pressure.

PRES	**PRES > 0**	Pressure
	PRES ≤ 0	Pressure drop (Default=0)
NPHASE	Number of phases in MIXED substream:	
	NPHASE = 1	One-phase calculation
	NPHASE = 2	Two-phase flash (Default)
	NPHASE = 3	Three-phase flash
PHASE	Specifies the phase when NPHASE=1:	
	PHASE = V	Vapor (Default)
	PHASE = L	Liquid
	PHASE = S	Solid. Use for electrolytes system only.
MAXIT	Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	
TOL	Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	

STREAM-FRAC Use to specify the fraction of the inlet stream going to an outlet stream. For a substream of type MIXED or CISOLID, the basis is assumed to be MOLE. For a substream of type NC, the basis is assumed to be MASS.

ssid	Substream ID (Default=MIXED)
sid	Outlet stream ID
frac	Split fraction

STREAM-MOLE-FLOW Use to specify the molar flow rate of an outlet stream. You cannot use this specification for a substream of type NC.

ssid	Substream ID (Default=MIXED)
sid	Outlet stream ID
flow	Molar flow rate

STREAM-MASS-FLOW Use to specify the mass flow rate of an outlet stream. You can use this specification for any type of substream.

ssid	Substream ID (Default=MIXED)
sid	Outlet stream ID
flow	Mass flow rate

STREAM-STDVOL-FLOW Use to specify the standard liquid-volume flow rate of an outlet stream. You can only use this specification for substreams of type MIXED.

sid	Outlet stream ID
flow	Standard liquid-volume flow rate

FRAC Use to specify the fraction of components in the inlet stream going to an outlet stream.

ssid	Substream ID (Default=MIXED)
sid	Outlet stream ID
cid-list	List of component IDs

frac-list ..... List of split fractions corresponding to *cid-list*

basis-FLOW Use to specify the flow rates of components in an outlet stream on a MOLE, MASS, or STDVOL basis. For substreams of type NC, only MASS basis is allowed. For substreams of type CISOLID, only MOLE and MASS bases are allowed.

ssid ..... Substream ID (Default=MIXED)

sid ..... Outlet stream ID

cid-list ..... List of component IDs

flow-list ..... List of component flow rates corresponding to *cid-list*

MOLE-FRAC Use to specify the mole fractions of components in an outlet stream. You cannot use this specification for a substream of type NC.

ssid ..... Substream ID (Default=MIXED)

sid ..... Outlet stream ID

cid-list ..... List of component IDs

frac-list ..... List of component mole fractions corresponding to *cid-list*

MASS-FRAC Use to specify the mass fractions of components in a substream of an outlet stream. You can use this specification for any type of substream.

ssid ..... Substream ID (Default=MIXED)

sid ..... Outlet stream ID

cid-list ..... List of component IDs

frac-list ..... List of component mass fractions corresponding to *cid-list*

FLASH-SPECS Use to specify the conditions of the outlet streams. The default is a TP flash using the block pressure and temperature.

sid ..... Stream ID

TEMP ..... Temperature

PRES ..... Pressure

DELT ..... Temperature difference

VFRAC ..... Molar vapor fraction. Enter 0.0 for bubble point, 1.0 for dew point. For subcooled liquid or superheated vapor, use TEMP and PRES specifications.

NPHASE ..... Number of phases in MIXED substream:

NPHASE = 1	One-phase calculation
NPHASE = 2	Two-phase flash (Default)
NPHASE = 3	Three-phase flash

PHASE ..... Specifies the phase when NPHASE=1:

PHASE = V	Vapor (Default)
PHASE = L	Liquid
PHASE = S	Solid. Use for electrolytes system only.

FREE-WATER ..... Use to override the free-water option established by the SIM-OPTIONS paragraph. (See Chapter 45.) Or use it to override the BLOCK-OPTIONS sentence of the BLOCK paragraph. (See Chapter 11.)

FREE-WATER = NO	Does not perform free-water calculations
FREE-WATER = YES	Performs free-water calculations

MAXIT ..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

TOL ..... Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

KODE ..... **KODE=NOFLASH** Suppresses flash calculations (Default=performs flash calculations)

T-EST ..... Temperature estimate for the outlet stream. Use to aid convergence when PRES and VFRAC are specified.

P-EST ..... Pressure estimate for the outlet stream. Use to aid convergence when TEMP and VFRAC are specified.

UTILITY Use to specify an optional utility to provide heating or cooling duty.

UTILITY-ID ..... Utility ID.

Accessing Variables in SEP2

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following table lists variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	ID2	Element
PARAM	PRES, MAXIT, TOL	—	—	—
STREAM-FRAC	FRAC	ssid	sid	—
STREAM- MOLE-FLOW	FLOW	ssid	sid	—
STREAM- MASS-FLOW	FLOW	ssid	sid	—
STREAM- STDVOL-FLOW	FLOW	MIXED	sid	—
FRAC	FRACS	ssid	sid	†
basis-FLOW	FLOWS	ssid	sid	†
MOLE-FRAC	FRACS	ssid	sid	†
MASS-FRAC	FRACS	ssid	sid	†
FLASH-SPECS	TEMP, PRES, DELT, VFRAC, T-EST, P-EST, MAXIT, TOL	sid	—	—

† Position of a component in the COMPS cid-list.

Block Results

Description	Sentence	Variable
Heat duty	RESULTS	QCALC

13 Flashes, Heaters, and Heat Exchangers

This chapter describes the input language for models that simulate flash and heat exchange operations, including models you can use as interfaces to the B-JAC thermal design programs and the HTRI IST program. You can generate heating or cooling curve tables for all models described in this chapter. The models are:

Model	Description	Purpose	Use
HEATER	Heater or cooler	Determines thermal and phase conditions	Heaters, coolers, valves. Pumps and compressors, when work-related results are not needed. One or two outlet material streams (second for optional water decant stream).
FLASH2	Two-outlet flash	Determines thermal and phase conditions	Flashes, evaporators, knockout drums, and single stage separators. Two or three outlet material streams (first for vapor, second for liquid, third for optional water decant stream).
FLASH3	Three-outlet flash	Determines thermal and phase conditions	Decanters, single-stage separators with two liquid phases. Three outlet material streams (first for vapor, second for first-liquid, third for second-liquid).
DECANTER	Liquid-liquid decanter	Determines thermal and phase conditions	Decanters, single-stage separators with two liquid phases and no vapor phase
HEATX	Two-stream heat exchanger	Exchange heat between two streams	Two-stream heat exchangers. Rating shell and tube heat exchangers when geometry is known.
MHEATX	Multi-stream heat exchanger	Exchange heat between any number of streams	Multiple hot and cold stream heat exchangers. Two-stream heat exchangers. LNG exchangers.
HXFLUX	Heat transfer calculation using convective heat transfer	Perform heat transfer calculations between a heat source and a heat sink	Two single-sided heat exchangers
HETRAN	Shell and tube heat exchanger	Provides interface to the B-JAC Hetran shell and tube heat exchanger program	Shell and tube heat exchangers, including kettle reboilers

continued

Flashes, Heaters, and Heat Exchanger Models (continued)

Model	Description	Purpose	Use
AEROTRAN	Air-cooled heat exchanger	Provides interface to the B-JAC Aerotran air-cooled heat exchanger program	Cross-flow heat exchangers, including air coolers
HTRIXIST	Shell and tube heat exchanger	Provides interface to HTRI's XIST shell and tube heat exchanger program	Shell and tube heat exchangers, including kettle reboilers

HEATER: Heater/Cooler

Input Language for HEATER

```
BLOCK    blockid    HEATER
PARAM    keyword=value
```

Keywords:

TEMP PRES VFRAC DUTY DELT DEGSUB DEGSUP

Optional keywords:

NPHASE PHASE MAXIT TOL T-EST P-EST

```
HCURVE    curveno    keyword=value
```

Optional keywords:

INDEP-VAR LIST NPOINT INCR HEADING PROPERTIES PRES-PROFILE PDROP PRINT-PLOT HIGH-PRECISION LINES X-SCALE Y-SCALE WIDE GRID INTERPOLATE

```
UTILITY    UTILITY-ID=utilityid
```

Input Language Description for HEATER

PARAM Use to specify outlet conditions of the heater.

TEMP..... Temperature

PRES..... **PRES > 0** Pressure

PRES ≤ 0 Pressure drop (Default=0)

VFRAC..... Molar vapor fraction. Enter 0.0 for bubble point, 1.0 for dew point. For subcooled or superheated vapor use TEMP, DEGSUB, or DEGSUP specifications. VFRAC is allowed only when NPHASE >1.

DUTY..... Heat duty

DELT ..... Temperature change

DEGSUB ..... Degrees of subcooling

DEGSUP ..... Degrees of superheat

NPHASE ..... Number of phases in MIXED substream:

NPHASE=1 One-phase calculation

NPHASE=2 Two-phase flash (Default)

NPHASE=3 Three-phase flash

PHASE..... Specifies the phase when NPHASE=1:

PHASE=V Vapor (Default)

PHASE=L Liquid

PHASE=S Solid. Use for electrolytes system only.

MAXIT..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

TOL..... Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

T-EST ..... Temperature estimate. Use to aid convergence when PRES and either VFRAC or DUTY are specified.

P-EST ..... Pressure estimate. Use to aid convergence when temperature (one of TEMP, DELT, DEGSUB, or DEGSUP) and either VFRAC or DUTY are specified.

HCURVE Use to generate heating or cooling curve tables and plots. See Chapter 11 for a description of the input keywords.

UTILITY Use to specify an optional utility to provide heating or cooling duty.

UTILITY-ID ..... Utility ID.

Accessing Variables in HEATER

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1
PARAM	TEMP, PRES, VFRAC, DUTY, DELT, DEGSUB, DEGSUP, MAXIT, TOL, T-EST, P-EST	—
HCURVE	NPOINT, INCR, PDROP	curveno

Block Results

Description	Sentence	Variable
Heat duty	PARAM	QCALC
Net heat duty	RESULTS	NET-DUTY

FLASH2: Two-Outlet Flash

Input Language for FLASH2

```
BLOCK    blockid    FLASH2
PARAM    keyword=value
```

Keywords:

TEMP PRES VFRAC DUTY

Optional keywords:

NPHASE ENTRN MAXIT TOL T-EST P-EST

```
FRAC     ssid    frac
HCURVE   curveno   keyword=value
```

Optional keywords:

INDEP-VAR LIST NPOINT INCR HEADING PROPERTIES PRES-PROFILE PDROP PRINT-PLOT HIGH-PRECISION LINES X-SCALE Y-SCALE WIDE GRID INTERPOLATE

```
UTILITY    UTILITY-ID=utilityid
```

Input Language Description for FLASH2

PARAM

Use to specify outlet conditions of the flash. You must supply two of the following variables: temperature, pressure, vapor fraction, or heat duty. FLASH2 accepts any combination, except vapor fraction and heat duty.

TEMP		Temperature
PRES	**PRES > 0**	Pressure
	PRES ≤ 0	Pressure drop (Default=0)
VFRAC		Molar vapor fraction. Enter 0.0 for bubble point, 1.0 for dew point. For subcooled liquid or superheated vapor, use TEMP and PRES specifications.
DUTY		Heat duty
NPHASE	**NPHASE=2**	Two-phase flash (Default)
	NPHASE=3	Three-phase flash
ENTRN		Fraction of liquid entrained in vapor stream (Default=0)
MAXIT		Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)
TOL		Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)
T-EST		Temperature estimate. Use to aid convergence when PRES and either VFRAC or DUTY are specified.

P-EST ..... Pressure estimate. Use to aid convergence when TEMP and either VFRAC or DUTY are specified.

FRAC Use to specify solid entrainment in vapor stream for each substream.

ssid ..... Substream ID

frac ..... Fraction of total inlet solids in the specified substream, placed into the corresponding substream of the vapor outlet stream

HCURVE Use to generate heating or cooling curve tables and plots. See Chapter 11 for a description of the input keywords.

UTILITY Use to specify an optional utility to provide heating or cooling duty.

UTILITY-ID ..... Utility ID.

Accessing Variables in FLASH2

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1
PARAM	TEMP, PRES, VFRAC, DUTY, ENTRN, MAXIT, TOL, T-EST, P-EST	—
FRAC	FRAC	ssid
HCURVE	NPOINT, INCR, PDROP	curveno

Block Results

Description	Sentence	Variable
Heat duty	PARAM	QCALC
Net heat duty	PARAM	NET-DUTY

FLASH3: Three-Outlet Flash

Input Language for FLASH3

```
BLOCK    blockid    FLASH3
PARAM    keyword=value
```

Keywords:

TEMP PRES VFRAC DUTY

Optional keywords:

L2-COMP MAXIT TOL T-EST P-EST

```
ENTRN   liqno   entrn / . . .
FRAC    ssid    keyword=value
```

Keywords:

VAPOR LIQUID1

```
HCURVE   curveno   keyword=value
```

Optional keywords:

INDEP-VAR LIST NPOINT INCR HEADING PROPERTIES PRES-PROFILE PDROP PRINT-PLOT HIGH-PRECISION LINES X-SCALE Y-SCALE WIDE GRID INTERPOLATE

```
UTILITY   UTILITY-ID=utilityid
```

Input Language Description for FLASH3

PARAM

Use to specify outlet conditions of the flash. You must specify two of the following variables: temperature, pressure, vapor fraction, or heat duty. FLASH3 accepts any combination, except vapor fraction and heat duty. You can differentiate the two liquid streams by defining a key component.

TEMP		Temperature
PRES	**PRES > 0**	Pressure
	PRES ≤ 0	Pressure drop (Default=0)
VFRAC		Molar vapor fraction. Enter 0.0 for bubble point, 1.0 for dew point. For subcooled liquid or superheated vapor, use TEMP and PRES specifications.
DUTY		Heat duty
L2-COMP		Key component ID. The liquid phase with the larger mole fraction of the key component is placed in the second-liquid stream. If you do not specify a key component, the liquid phase with the higher density is placed in the second-liquid stream. If only one liquid phase exists, it is placed in the first-liquid stream.
MAXIT		Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)
TOL		Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)
T-EST		Temperature estimate. Use to aid convergence when PRES and either VFRAC or DUTY are specified.
P-EST		Pressure estimate. Use to aid convergence when TEMP and either VFRAC or DUTY are specified.

ENTRN

Use to specify the fraction of each liquid phase that is entrained in the vapor.

liqno	**1**	First-liquid phase
	2	Second-liquid phase
entrn		Fraction of the liquid phase entrained in the vapor stream

FRAC

Use to specify solid entrainment in vapor and liquid streams for each substream.

ssid	Substream ID

VAPOR ..... Fraction of total inlet solids in the specified substream, placed in the corresponding substream of the vapor outlet stream

LIQUID1 ..... Fraction of total inlet solids in the specified substream, placed in the corresponding substream of the first-liquid outlet stream

HCURVE Use to generate heating or cooling curve tables and plots. See Chapter 11 for a description of the input keywords.

UTILITY Use to specify an optional utility to provide heating or cooling duty.

UTILITY-ID ..... Utility ID.

Accessing Variables in FLASH3

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1
PARAM	TEMP, PRES, VFRAC, DUTY, MAXIT, TOL, T-EST, P-EST	—
ENTRN	ENTRN	liqno
FRAC	VAPOR, LIQUID1	ssid
HCURVE	NPOINT, INCR, PDROP	curveno

Block Results

Description	Sentence	Variable
Heat duty	PARAM	QCALC
Net heat duty	PARAM	NET-DUTY

DECANTER: Liquid-Liquid Decanter

Input Language for DECANTER

```
BLOCK    blockid    DECANTER
PARAM    keyword=value
```

Keywords:

PRES TEMP DUTY L2-COMPS

Optional keywords:

L2-CUTOFF KLL-CORR BASIS LL-METH MAXIT TOL

```
COEF-KLL   cid   coeffa   coeffb   coeffc   coeffd  / ...
SEP-EFF    cid   eff  / ...
SOLID-FRAC   sid   frac  / ...
PHASE-PROPS    keyword=value
```

Optional keywords:

L1OPSET L1SOLU-WATER L1HENRY-COMP L1CHEMISTRY
L2OPSET L2SOLU-WATER L2HENRY-COMP L2CHEMISTRY

HCURVE curveno *keyword=value*

Option keywords:

INDEP-VAR LIST NPOINT INCR HEADING PROPERTIES
PRES-PROFILE PDROP PRINT-PLOT HIGH-PRECISION LINES
X-SCALE Y-SCALE WIDE GRID INTERPOLATE

SUBROUTINE subrname
USER-VEC *keyword=value*

Keywords:

NINT NREAL NIWORK NWORK KLL-INT KLL-REAL

UTILITY UTILITY-ID=*utilityid*

Input Language Description for DECANTER

PARAM

Use to specify decanter outlet conditions. You must specify pressure. You must specify either temperature or duty. You can differentiate the two outlet liquid streams by specifying the key components in the second-liquid phase. You can also specify the phase-splitting calculation method and convergence parameters.

PRES	**PRES > 0**	Pressure
	PRES ≤ 0	Pressure drop (Default=0)
TEMP	Temperature	
DUTY	Heat duty	
L2-COMPS	Key component IDs. The liquid phase with the larger sum of mole fractions of the key components is placed in the second-liquid stream. If you do not specify L2-COMPS, the liquid phase with the higher density is placed in the second-liquid stream. If only one liquid phase exists, the L2-CUTOFF value determines into which stream the single-outlet liquid phase is placed.	
L2-CUTOFF	Use only if L2-COMPS is specified, and only one liquid phase is present. It determines into which stream the single-outlet liquid phase is placed. If the sum of mole fractions of components specified as L2-COMPS is larger than the L2-CUTOFF value, the liquid is placed in the second outlet stream. (Default=0.5)	
KLL-CORR	Correlation for distribution coefficients ($KLL=X_2/X_1$). If you do not specify KLL-CORR, KLL is computed from the property option set specified for the block.	
	KLL-CORR=SUBROUTINE	Uses user-supplied FORTRAN subroutine

KLL-CORR=POLYNOMIAL Uses built-in logarithmic polynomial in terms of temperature. The BASIS keyword defines the basis of the computed KLL values.

BASIS ..... Basis of distribution coefficient (KLL) when KLL-CORR=POLYNOMIAL:

BASIS=MOLE Mole basis (Default)

BASIS=MASS Mass basis

LL-METH ..... Phase-splitting calculation method:

LL-METH=EQ-SOLVE Equates liquid fugacities (Default)

LL-METH=GIBBS Gibbs free-energy minimization

MAXIT..... Maximum number of iterations (Default=30)

TOL..... Convergence tolerance (Default=$1x10^{-4}$)

COEF-KLL

Use to specify coefficients for the built-in polynomial KLL expression. COEF-KLL is only allowed when KLL-CORR=POLYNOMIAL.

cid..... Component ID

coeffa, coeffb, coeffc, coeffd ..... Coefficients of the KLL expression, which is defined as:

$$\ln(KLL) = coeffa + \frac{coeffb}{T} + coeffc \times \ln(T) + coeffd \times T$$

Where:
KLL = Liquid-liquid equilibrium K-value
T = Temperature in Kelvin

Enter an asterisk (*) if value is missing

SEP-EFF

Use to enter values for separation efficiency by component. The following expression defines efficiency: $X_i^{L_2} = (eff)_i KLL_i X_i^{L_1}$

Where:

KLL = Liquid-liquid equilibrium K-value

X^{L_1} = Liquid1 mole fraction

X^{L_2} = Liquid2 mole fraction

i = Component index

cid..... Component ID

eff..... Efficiency (Default=1.0)

SOLID-FRAC

Use to specify solid entrainment in the first outlet liquid phase.

sid..... Substream ID

frac..... Fraction of total inlet solids in the specified substream. This fraction is placed into the corresponding substream of the first-liquid outlet stream. (Default=0)

PHASE-PROPS

Use to override property options for each of the two outlet streams.

L1OPSET..... Option set name for the first-liquid phase

L1SOLU-WATER..... Method for calculating K-value of water. (See Chapter 8.)

L1HENRY-COMP..... Henry's law component list ID for the first-liquid phase. (See Chapter 8.)

L1CHEMISTRY ..... Chemistry ID for the first-liquid phase. (See Chapter 5.)

L2OPSET ..... Option set name for the second-liquid phase

L2SOLU-WATER ..... Method for calculating K-value of water for the second-liquid phase.
(See Chapter 8.)

L2HENRY-COMP ..... Henry's law component list ID for the second-liquid phase.
(See Chapter 8.)

L2CHEMISTRY ..... Chemistry ID for the second-liquid phase. (See Chapter 5.)

HCURVE

Use to generate heating or cooling curve tables and plots for decanter. See Chapter 11 for a description of input keywords.
Note: INDEP-VAR=VFRAC is not allowed for DECANTER.

SUBROUTINE

Use to specify user-supplied KLL subroutine. SUBROUTINE is only allowed when KLL-CORR=SUBROUTINE. For details on writing a user-supplied KLL subroutine, see *Aspen Plus User Models*, Chapter 16.

subrname ..... User-supplied FORTRAN subroutine name

USER-VEC

Use to define the length of arrays for the user-supplied KLL subroutine.

NINT ..... Length of integer parameter array

NREAL ..... Length of real parameter array

NIWORK ..... Length of integer workspace array

NWORK ..... Length of real workspace array

KLL-INT ..... List of integer values for integer parameter array

KLL-REAL ..... List of real values for real parameter array

UTILITY

Use to specify an optional utility to provide heating or cooling duty.

UTILITY-ID ..... Utility ID.

Accessing Variables in DECANTER

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1
PARAM	PRES, TEMP, DUTY, L2-CUTOFF, MAXIT, TOL	—
COEF-KLL	COEFFA, COEFFB, COEFFC, COEFFD	cid
SOLID-FRAC	FRAC	sid
HCURVE	NPOINT, INCR, PDROP	curveno

Block Results

Description	Sentence	Variable
Outlet temperature	SCAL-RESULTS	TCALC
Duty	SCAL-RESULTS	QCALC
Net heat duty	SCAL-RESULTS	NET-DUTY

HEATX: Two-Stream Heat Exchanger

Input Language for HEATX

```
BLOCK    blockid    HEATX
PARAM    keyword=value
```

Keywords:

CALC-METHOD CALC-TYPE T-HOT T-COLD DUTY AREA
DELT-HOT DELT-COLD DEGSUB-HOT DEGSUP-COLD
VFRAC-HOT VFRAC-COLD DECR-HOT INCR-COLD MIN-OUT-TAPP

Optional keywords:

TYPE NUM-SHELLS U-OPTION USER-SUBR-OPT F-OPTION FT-MIN
LMTD-CORRECT PRES-HOT PRES-COLD TUBE-DP-FCORR TUBE-DP-HCORR
P-UPDATE NPOINTS ALLOW-TCROSS MAXIT ALGORITHM Q-ESTIMATE
TEMP-TOL PRES-TOL AREA-TOL MIN-TAPP SILVER-GHALY
MAX-NSHELLS MIN-FLS-PTS MIN-HRC-PTS SCUT-INTVLS CALC-NSHELLS
USE-OLD-NTU FC-USE-AVTD UA

```
FEEDS    HOT=sid    COLD=sid
PRODUCTS    HOT=sid    COLD=sid
DECANT-STREAMS    [HOT=sid]    [COLD=sid]
REFERENCE    utilityside=utilityid
```

Utility side specifications:

HOT-UTIL COLD-UTIL

```
HEAT-TR-COEF    keyword=value
```

Optional keywords:

U SCALE REF-SIDE FLOW-BASIS REF-VALUE EXPONENT
basis-RFLOW L-L B-L V-L L-B B-B V-B L-V B-V V-V

```
HOT-SIDE    keyword=value
COLD-SIDE    keyword=value
```

Keywords:

SHELL-TUBE H-OPTION DP-OPTION

Optional keywords:

H-SCALE FLOW-BASIS REF-VALUE EXPONENT basis-RFLOW H H-L
H-B H-V MAX-DP DP-SCALE FOUL-FACTOR

```
CROSSFLOW    keyword=value
```

Optional keywords:

TUBE-MIXED SHELL-MIXED

EQUIP-SPECS *keyword=value*

Optional keywords:

TUBE-NPASS TEMA-TYPE BAFFLE-TYPE ORIENTATION TUBE-FLOW SHELL-DIAM SHELL-BND-SP

TUBES *keyword=value*

Keywords:

TOTAL-NUMBER NUMBER-ROWS TUBE-TYPE LENGTH INSIDE-DIAM OUTSIDE-DIAM

Optional keywords:

NOMINAL-SIZE BWG WALL-THICK PITCH PATTERN MATERIAL TCOND

NOZZLES *keyword=value*

Optional keywords:

SNOZ-INDIAM SNOZ-OUTDIAM TNOZ-INDIAM TNOZ-OUTDIAM

SEGB-SHELL *keyword=value*

Optional keywords:

NBAFFLE NSEAL-STRIP TUBES-IN-WIN BAFFLE-CUT SHELL-BFL-SP TUBE-BFL-SP MID-BFL-SP IN-BFL-SP OUT-BFL-SP

RODB-SHELL *keyword=value*

Optional keywords:

NBAFFLE MID-BFL-SP RING-INDIAM RING-OUTDIAM ROD-DIAM ROD-LENGTH

FINS *keyword=value*

Keywords:

AREA-RATIO EFFICIENCY

Optional keywords:

ROOT-DIAM NPER-LENGTH THICKNESS HEIGHT

HETRAN-PARAM *keyword=value*

Keywords:

INPUT-FILE

Optional keywords:

SAV-HOT-STRM SAV-CLD-STRM SAV-DSG-PARM SAV-ANA-PARM

HOT-PCURVE *keyword=value*

Optional keywords:

GENERATE UPDATE INDP-DEV TYPE

COLD-PCURVE *keyword=value*

Optional keywords:

GENERATE UPDATE INDP-DEV TYPE

BJAC-INPUTS *keyword=value*

Optional keywords:

HOT-FOULING HOT-FILM HOT-PFACTOR HOT-FFACTOR HOT-MAX-DP COLD-FOULING COLD-FILM COLD-PFACTOR COLD-FFACTOR COLD-MAX-DP FOUL-OPTION FOUL-RATIO

PROPERTIES opsetname *keyword=value* **[/ opsetname** *keyword=value* **]**

Optional keywords:

FREE-WATER SOLU-WATER HENRY-COMPS

FLASH-SPECS sid *keyword=value*

Optional keywords:

NPHASE PHASE FREE-WATER MAXIT TOL

HOT-HCURVE curveno *keyword=value*
COLD-HCURVE curveno *keyword=value*

Optional keywords:

INDEP-VAR LIST NPOINT INCR HEADING PROPERTIES PRES-PROFILE PDROP PRINT-PLOT HIGH-PRECISION LINES X-SCALE Y-SCALE WIDE GRID INTERPOLATE

REPORT PROFILE
SUBROUTINE *keyword=value*

Optional keywords:

HEAT-TR-COEF LMTD-CORRECT TUBE-DP-HLDP TUBE-DP-PDRP

USER-VECS

Optional keywords:

NINTU NREALU NIWRKU NWRKU NINTF NREALF NIWRKF NWRKF NINTH NREALH NIWRKH NWRKH NINTT NREALT NIWRKT NWRKT

USER-INT-U value-list
USER-REAL-U value-list
USER-INT-F value-list
USER-REAL-F value-list
USER-INT-H value-list
USER-REAL-H value-list
USER-INT-T value-list
USER-REAL-T value-list

Input Language Description for HEATX

blockid ..... Block ID

PARAM Use to enter the heat exchanger calculation specifications and convergence parameters.

CALC-METHOD ..... Method of modeling of heat exchanger

CALC-METHOD = SHORTCUT	Perform shortcut design calculations (Default)
CALC-METHOD = DETAILED	Perform rigorous rating calculations for the specified shell-and-tube heat exchanger. You must specify exchanger geometry (EQUIP-SPECS, TUBES, NOZZLES, and SEGB-SHELL, RODB-SHELL, or FINS when appropriate) when using this option.
CALC-METHOD = HETRAN/TASC-RIG	Perform rigorous design, rating, or simulation calculations using Aspen Hetran or HTFS TASC.
CALC-METHOD = AEROTRAN-RIG	Perform rigorous design, rating, or simulation calculations using Aspen Aerotran.

CALC-TYPE ..... Type of heat exchanger calculation.

CALC-TYPE = DESIGN	Select the geometry based on process conditions
CALC-TYPE = RATING	Determine if exchanger is over or under-surfaced based on the given geometry
CALC-TYPE = SIMULATION	Determine outlet conditions assuming surface area is fully utilized

T-HOT ..... Outlet temperature of the hot stream

T-COLD ..... Outlet temperature of the cold stream

DUTY..... Exchanger heat duty

AREA..... Heat transfer area

UA..... User-specified UA value

DELT-HOT ..... Temperature approach at the hot stream outlet

DELT-COLD ..... Temperature approach at the cold stream outlet

DEGSUB-HOT ..... Degrees of subcooling of hot stream outlet

DEGSUP-COLD..... Degrees of superheat of cold stream outlet

VFRAC-HOT..... Vapor fraction of hot stream outlet

VFRAC-COLD ..... Vapor fraction of cold stream outlet

DECR-HOT..... Temperature decrease of the hot stream

INCR-COLD ..... Temperature increase of the cold stream

MIN-OUT-TAPP ..... Hot/cold outlet temperature approach

TYPE ..... Overall direction of flow in the exchanger:

TYPE= COUNTERCURRENT	Countercurrent heat exchanger (Default)
TYPE=COCURRENT	Cocurrent heat exchanger
TYPE=MULTIPASS	Multiple tube passes. Simulates a system of identical one-shell-pass, multiple-tube-pass heat exchangers in series.

NUM-SHELLS..... Number of heat exchangers in series. Allowed only when TYPE=MULTIPASS. (Default=1)

U-OPTION ..... Overall heat transfer coefficient (U) calculation option:

	U-OPTION=CONSTANT	Uses user-specified value for heat transfer coefficient (Default)
	U-OPTION=PHASE	Uses user-specified phase-based values for heat transfer coefficient
	U-OPTION=POWER-LAW	Uses power-law expression to calculate heat transfer coefficient
	U-OPTION=FILM-COEF	Calculates heat transfer coefficient from film coefficients
	U-OPTION=GEOMETRY	Calculates heat transfer coefficient from the user-supplied exchanger geometry
	U-OPTION=USER-SUBR	Uses heat transfer coefficient returned by a user-supplied subroutine

USER-SUBR-OPT ..... Calculation option for user heat transfer coefficient user-supplied subroutine:

USER-SUBR-OPT= SINGLE	Calculates a single heat transfer coefficient at the average stream conditions (Default)
USER-SUBR-OPT= POINTWISE	Calculates heat transfer coefficients for each point in the area integration

F-OPTION ..... Calculation option for Log-Mean Temperature Difference (LMTD) correction factor:

F-OPTION=CONSTANT	Uses a user-specified value for the LMTD correction factor (Default)
F-OPTION=GEOMETRY	Calculates the LMTD correction factor from the exchanger flow configuration and stream conditions
F-OPTION=USER-SUBR	Uses a user-supplied subroutine to calculate the LMTD correction factor
F-OPTION=CALCULATED	Calculates the LMTD correction factor for a system of identical one-shell-pass, multiple-tube-pass exchangers in series. Required for and allowed only when TYPE=MULTIPASS.

FT-MIN..... Minimum allowed value of the LMTD correction factor for TYPE=MULTIPASS. If specified, and the calculated LMTD correction factor is less than FT-MIN, HEATX issues a warning.

LMTD-CORRECT..... User-specified LMTD correction factor (Default=1.0)

PRES-HOT	**PRES-HOT > 0**	Outlet pressure of hot stream
	PRES-HOT ≤ 0	Pressure drop of hot stream (Default=0 N/m^2)
PRES-COLD	**PRES-COLD > 0**	Outlet pressure of cold stream
	PRES-COLD ≤ 0	Pressure drop of cold stream (Default=0 N/m^2)

TUBE-DP-FCORR ..... Tube-side frictional pressure-drop correlation:

TUBE-DP-FCORR=AWR	Angel-Welchon-Ros correlation
TUBE-DP-FCORR= BEGGS-BRILL	Beggs-Brill correlation (Default)
TUBE-DP-FCORR= DARCY	Darcy's law
TUBE-DP-FCORR= DUKLER	Dukler correlation
TUBE-DP-FCORR= H-BROWN	Hagedorn-Brown correlation
TUBE-DP-FCORR= LOCK-MART	Lockhart-Martinelli correlation

	TUBE-DP-FCORR=ORKI	Orkiszewski correlation
	TUBE-DP-FCORR=SLACK	Slack correlation
	TUBE-DP-FCORR= USER-SUBR	Uses a user-supplied subroutine to calculate pressure-drop in two-phase flow
TUBE-DP-HCORR	Tube-side holdup pressure-drop correlation:	
	TUBE-DP-HCORR=AWR	Angel-Welchon-Ros correlation
	TUBE-DP-HCORR= BEGGS-BRILL	Beggs-Brill correlation (Default)
	TUBE-DP-HCORR=EATON	Eaton correlation
	TUBE-DP-HCORR= FLANIGAN	Flanigan correlation
	TUBE-DP-HCORR= H-BROWN	Hagedorn-Brown correlation
	TUBE-DP-HCORR=HOOG	Hoogendorn correlation
	TUBE-DP-HCORR=HUGH	Hughmark correlation
	TUBE-DP-HCORR= LOCK-MART	Lockhart-Martinelli correlation
	TUBE-DP-HCORR=ORKI	Orkiszewski correlation
	TUBE-DP-HCORR=SLACK	Slack correlation
	TUBE-DP-HCORR= USER-SUBR	Uses a user-supplied subroutine to calculate liquid holdup in two-phase flow
P-UPDATE	Flag to control pressure convergence:	
	P-UPDATE=YES	Converges shellside and tube-side pressure drops (Default)
	P-UPDATE=NO	Calculates pressure drops only once. Does not apply calculated pressure drops to outlet streams.
NPOINTS	The number of intervals per heat transfer zone for area integration (Default=1)	
ALLOW-TCROSS	Flag to control model behavior when a temperature crossover is detected:	
	ALLOW-TCROSS=YES	Takes no special action if a temperature crossover occurs
	ALLOW-TCROSS=NO	Does not allow a temperature crossover. If a temperature crossover occurs, HEATX changes the specification to a temperature approach using the minimum approach temperature and recomputes the block. (Default)
MAXIT	Maximum number of iterations for the block convergence (Default=20)	
ALGORITHM	Algorithm used to converge the heat exchanger calculations:	
	ALGORITHM=NEWTON	Uses the Newton method to converge all variables simultaneously
	ALGORITHM=BROYDEN	Uses a tearing approach with a subset of variables converged by the Broyden method (Default)
Q-ESTIMATE	Initial estimate of duty for area convergence	
TEMP-TOL	Temperature error tolerance (Default=$1x10^{-2}$ K)	
PRES-TOL	Pressure error tolerance (Default=100 N/m^2)	
AREA-TOL	Area error tolerance (Default=$1x10^{-2}$ m^2)	
MIN-TAPP	Minimum approach temperature (Default=1.0 K)	

SILVER-GHALY..... Flag to correct for the presence of non-condensable components:

SILVER-GHALY=YES	Uses the Silver-Ghaly method to correct for the presence of non-condensable components (Default)
SILVER-GHALY=NO	Does not correct for the presence of non-condensable components

MAX-NSHELLS..... Maximum number of multipass exchangers in series

MIN-FLS-PTS ..... Minimum number of flash points used to determine the temperature/heat load profiles

MIN-HRC-PTS ..... The number of intervals between flash points

SCUT-INTVLS..... Whether to use shortcut LMTD interval analysis which divides the hot and cold side temperature/heat profile into intervals and provides more accurate overall LMTD, heat transfer coefficient, and required area results.

SCUT-INTVLS=YES	Use shortcut LMTD interval analysis
SCUT-INTVLS=NO	Do not use shortcut LMTD interval (Default)

CALC-NSHELLS..... Whether to determine the number of exchangers in series required to meet a specified minimum LMTD correction factor. Allowed only when TYPE=MULTIPASS.

CALC-NSHELLS=YES	Determine number of exchangers in series
CALC-NSHELLS=NO	Do not determine number of exchangers in series (Default)

USE-OLD-NTU ..... Correlation to use for computing FT for TEMA E shells.

USE-OLD-NTU=YES	Use old correlation
USE-OLD-NTU=NO	Use new correlation (Default)

FC-USE-AVTD..... Method to determine MTD when film coefficients are computed.

FC-USE-AVTD=YES	Use local midpoints of each interval
FC-USE-AVTD=NO	Use terminal points of each interval (Default)

FEEDS, PRODUCTS, DECANT-STREAMS

Use to identify inlet and outlet streams. You must identify hot and cold inlets and outlets and any water decant streams. Exception: When a utility is specified for one side of the exchanger in the REFERENCE sentence, do not specify inlet and outlet streams for that side.

HOT ..... Stream ID for the hot-side

COLD..... Stream ID for the cold-side

REFERENCE

Use to specify a utility for one side of the heat exchanger. Specify only one keyword and do not specify inlets and outlets for that side in the FEEDS and PRODUCTS sentences.

HOT-UTIL..... Utility ID for the hot side

COLD-UTIL..... Utility ID for the cold side

HEAT-TR-COEF

Use to specify the heat transfer coefficient.

U..... User-supplied heat transfer coefficient (Default=850.0 W/m^2-K)

SCALE ..... Correction factor to be applied to the rigorously computed heat transfer coefficient (Default=1.0)

REF-SIDE ..... Stream side (hot or cold) where flow will be used as the reference flow in the power-law expression for U (Default=HOT)

FLOW-BASIS..... Flow basis for reference flow in power-law expression for U:

FLOW-BASIS=MOLE	Molar basis (Default)

	FLOW-BASIS=MASS	Mass basis
	FLOW-BASIS=STDVOL	Standard-liquid-volume basis

REF-VALUE ..... Factor in a power-law expression for U of the form: U=REF-VALUE*(flow/REF-FLOW)**EXPONENT (Default=850.0 W/m^2-K)

EXPONENT ..... Exponent in the power-law expression for U (Default=1.0)

basis-RFLOW ..... Reference flow for power-law expression in MOLE, MASS, or STDVOL basis

L-L ..... Phase-based heat transfer coefficient used when both the hot stream and cold streams are liquid (Default=850 W/m^2-K)

B-L ..... Phase-based heat transfer coefficient used when the hot stream is two-phase and the cold stream is liquid (Default=850 W/m^2-K)

V-L ..... Phase-based heat transfer coefficient used when the hot stream is vapor and the cold stream is liquid (Default=850 W/m^2-K)

L-B ..... Phase-based heat transfer coefficient used when the hot stream is liquid and the cold stream is two-phase (Default=850 W/m^2-K)

B-B ..... Phase-based heat transfer coefficient used when both the hot and cold streams are two-phase (Default=850 W/m^2-K)

V-B ..... Phase-based heat transfer coefficient used when the hot stream is vapor and the cold stream is two-phase (Default=850 W/m^2-K)

L-V ..... Phase-based heat transfer coefficient used when the hot stream is liquid and the cold stream is vapor (Default=850 W/m^2-K)

B-V ..... Phase-based heat transfer coefficient used when the hot stream is two-phase and the cold stream is vapor (Default=850 W/m^2-K)

V-V ..... Phase-based heat transfer coefficient used when both the hot and cold streams are vapor (Default=850 W/m^2-K)

HOT-SIDE, COLD-SIDE

Use to enter the film coefficients, the shell and tube allocation of streams, and the fouling factors.

SHELL-TUBE ..... Side of the exchanger for the hot stream (Applies only to HOT-SIDE; Default=SHELL)

H-OPTION ..... Film coefficient (H) calculation flag:

H-OPTION=CONSTANT	Uses constant value for film coefficient (Default)
H-OPTION=PHASE	Uses phase-based coefficients for film coefficient
H-OPTION=POWER-LAW	Uses power-law expression for film coefficient
H-OPTION=GEOMETRY	Calculates film coefficient from exchanger geometry

DP-OPTION ..... Pressure drop calculation flag:

DP-OPTION=CONSTANT	Uses constant value for pressure drop (Default)
DP-OPTION=GEOMETRY	Calculates pressure drop from exchanger geometry

H-SCALE Correction factor to apply to the rigorously computed film coefficient (Default=1.0)

FLOW-BASIS Flow basis for reference flow:

FLOW-BASIS=MOLE	Uses molar flow for basis in power-law expression for H (Default)
FLOW-BASIS=MASS	Uses mass flow for basis in power-law expression for H
FLOW-BASIS=STDVOL	Uses standard liquid volume flow for basis in power-law expression for H

REF-VALUE Factor in a power-law expression for H of the form: H=REF-VALUE*(flow/REF-FLOW)**EXPONENT.

Allowed only when H-OPTION=POWER-LAW. (Default=1700.0 W/m^2-K)

EXPONENT Exponent in the power-law expression for H. Allowed only when H-OPTION=POWER-LAW. (Default=1.0)

basis-RFLOW Reference flow for power-law expression in MASS, MOLE, or STDVOL basis. Allowed only when H-OPTION=POWER-LAW.

H User-supplied film coefficient. Allowed only when H-OPTION=CONSTANT. (Default=1700.0 W/m^2-K)

H-L Phase-based film coefficient used when the stream is liquid. Allowed only when H-OPTION=PHASE. (Default=1700.0 W/m^2-K)

H-B Phase-based film coefficient used when the stream is two-phase. Allowed only when H-OPTION=PHASE. (Default=1700.0 W/m^2-K)

H-V Phase-based film coefficient used when the stream is vapor. Allowed only when H-OPTION=PHASE. (Default=1700.0 W/m^2-K)

MAX-DP Maximum pressure drop expressed as a fraction of the input pressure. Allowed only when H-OPTION=GEOMETRY. (Default=0.4)

DP-SCALE Correction factor to apply to the rigorously computed pressure drop. Allowed only when H-OPTION=GEOMETRY. (Default=1.0)

FOUL-FACTOR Fouling factor. Allowed only when H-OPTION=GEOMETRY. (Default=0.0)

CROSSFLOW

Use to specify flow patterns for crossflow exchangers.

TUBE-MIXED Flag indicating how the stream is mixed during flow through the tubes:

TUBE-MIXED=UNMIXED	Shell stream is radially unmixed during flow through the shell. (Default)
TUBE-MIXED= THROUGHOUT	Tube stream is radially mixed throughout during flow through the tubes.

SHELL-MIXED Flag indicating how the stream is mixed in the exchanger:

SHELL-MIXED=UNMIXED	Shell stream is radially unmixed during flow through the shell. (Default)
SHELL-MIXED= THROUGHOUT	Shell stream is radially mixed throughout during flow through the shell.

EQUIP-SPECS

Use to specify number of shells, number of passes, TEMA shell type, and other general physical exchanger parameters.

TUBE-NPASS Number of tube passes (Default=1)

TEMA-TYPE Standard TEMA shell type:

	TEMA-TYPE=E	TEMA E Shell (Default)
	TEMA-TYPE=F	TEMA F Shell
	TEMA-TYPE=G	TEMA G Shell
	TEMA-TYPE=H	TEMA H Shell
	TEMA-TYPE=J	TEMA J Shell
	TEMA-TYPE=X	TEMA X Shell
BAFFLE-TYPE	Type of shell baffle:	
	BAFFLE-TYPE=SEGMENTAL	Segmental baffles (Default)
	BAFFLE-TYPE=ROD	ROD baffles
ORIENTATION	Exchanger physical orientation:	
	ORIENTATION=HORIZONTAL	Shell is mounted horizontally (Default)
	ORIENTATION=VERTICAL	Shell is mounted vertically
TUBE-FLOW	Direction of tube-side flow for vertical exchangers:	
	TUBE-FLOW=UP	Tube-side stream enters from the bottom of the exchanger (Default)
	TUBE-FLOW=DOWN	Tube-side stream enters from the top of the exchanger
SHELL-DIAM	Inside shell diameter (Default is calculated)	
SHELL-BND-SP	Space between the shell and the tube bundle (Default is calculated)	

TUBES

Use to specify dimensions of the tube bundle.

TOTAL-NUMBER	Total number of tubes (Default is calculated)	
NUMBER-ROWS	Number of tube rows (Default is calculated)	
TUBE-TYPE	Type of tube:	
	TYPE=BARE	The tubes are bare (Default)
	TYPE=FINNED	The tubes are finned
LENGTH	Tube length between the tubesheets (Default is calculated)	
INSIDE-DIAM	Tube inside diameter (Default is calculated)	
OUTSIDE-DIAM	Tube outside diameter (Default is calculated)	
NOMINAL-SIZE	Outside diameter of the tubes in standard sizes:	
	NOMINAL-SIZE="0.25IN"	1/4 inch standard tubes
	NOMINAL-SIZE="0.375IN"	3/8 inch standard tubes
	NOMINAL-SIZE="0.5IN"	1/2 inch standard tubes
	NOMINAL-SIZE="0.625IN"	5/8 inch standard tubes
	NOMINAL-SIZE="0.75IN"	3/4 inch standard tubes
	NOMINAL-SIZE="0.875IN"	7/8 inch standard tubes
	NOMINAL-SIZE="1.0IN"	1 inch standard tubes (Default)
	NOMINAL-SIZE="1.25IN"	1 1/4 inch standard tubes
	NOMINAL-SIZE="1.5IN"	1 1/2 inch standard tubes
	NOMINAL-SIZE="2.0IN"	2 inch standard tubes
	NOMINAL-SIZE="2.5IN"	2 1/2 inch standard tubes

BWG..... Birmingham wire gauge. Use to specify the thickness of the tube wall in standard amounts. The available BWG values depend on the choice of NOMINAL-SIZE. You cannot enter BWG if you specified WALL-THICK.

BWG=7	0.180 inch wall thickness
BWG=8	0.165 inch wall thickness
BWG=9	0.150 inch wall thickness
BWG=10	0.134 inch wall thickness
BWG=11	0.120 inch wall thickness
BWG=12	0.109 inch wall thickness
BWG=13	0.095 inch wall thickness
BWG=14	0.083 inch wall thickness
BWG=15	0.072 inch wall thickness
BWG=16	0.065 inch wall thickness (Default)
BWG=17	0.058 inch wall thickness
BWG=18	0.049 inch wall thickness
BWG=19	0.042 inch wall thickness
BWG=20	0.035 inch wall thickness
BWG=21	0.032 inch wall thickness
BWG=22	0.028 inch wall thickness
BWG=23	0.025 inch wall thickness
BWG=24	0.022 inch wall thickness
BWG=25	0.020 inch wall thickness
BWG=26	0.018 inch wall thickness
BWG=27	0.016 inch wall thickness

WALL-THICK..... Thickness of the tube wall. You cannot enter WALL-THICK if you specified BWG.

PITCH..... Center-to-center distance between adjacent tubes (Default is calculated)

PATTERN..... Tube bank layout pattern perpendicular to shell-side fluid flow:

PATTERN=SQUARE	(90º pitch angle) (Default)
PATTERN= ROT-TRIANGLE	(60º pitch angle)
PATTERN=ROT-SQUARE	(45º pitch angle)
PATTERN=TRIANGLE	(30º pitch angle)

MATERIAL..... Tube material. See Table 13.1 for a list of tube materials. (Default=CARBON-STEEL)

TCOND..... Tube thermal conductivity

NOZZLES Use to specify dimensions of the exchanger nozzles.

SNOZ-INDIAM..... Diameter of the shell inlet nozzle (Default is calculated)

SNOZ-OUTDIAM..... Diameter of the shell outlet nozzle (Default is calculated)

TNOZ-INDIAM..... Diameter of the tube inlet nozzle (Default is calculated)

TNOZ-OUTDIAM..... Diameter of the tube outlet nozzle (Default is calculated)

SEGB-SHELL Use to specify dimensions of segmental baffle shells. Allowed only when BAFFLE-TYPE=SEGMENTAL.

NBAFFLE..... Total number of baffles in the shell (excluding flow dividers) (Default=2)

NSEAL-STRIP ..... Number of sealing strip pairs (Default=0)

TUBES-IN-WIN ..... Flag for tubes present in the baffle window: YES or NO (Default=YES)

BAFFLE-CUT ..... Baffle window height as a fraction of shell inside diameter (Default=0.25)

SHELL-BFL-SP ..... Space between the shell and the baffles (Default is calculated)

TUBE-BFL-SP..... Space between the tube holes and the baffle (Default is calculated)

MID-BFL-SP ..... Spacing between baffles (Default is calculated)

IN-BFL-SP..... Spacing between the tube-sheet and first baffle (Default is calculated)

OUT-BFL-SP ..... Spacing between the tube-sheet and last baffle (Default is calculated)

RODB-SHELL Use to specify dimensions of ROD baffle shells. Allowed only when BAFFLE-TYPE=ROD.

NBAFFLE ..... Total number of baffles in the shell (excluding flow dividers) (Default=2)

MID-BFL-SP ..... Spacing between baffles in the shell (Default is calculated)

RING-INDIAM..... Inside diameter of the baffle ring (Default is calculated)

RING-OUTDIAM ..... Outside diameter of the baffle ring (Default is calculated)

ROD-DIAM ..... Diameter of the support rods (Default is calculated)

ROD-LENGTH ..... Length of all support rods in a single baffle (Default is calculated)

FINS Use to specify the dimensions of tube fins. Allowed only when TUBE-TYPE=FINNED.

AREA-RATIO ..... Ratio of the total outside area of the finned tube to the inside tube area (Default is calculated)

EFFICIENCY ..... Efficiency of the finned tube (Default is calculated)

ROOT-DIAM ..... Finned tube root diameter (Default is calculated)

NPER-LENGTH..... Number of fins per unit length (Default is calculated)

THICKNESS..... Thickness of the fins (Default is calculated)

HEIGHT..... Height of the fins (Default is calculated)

HETRAN-PARAM Use to enter the B-JAC or HTFS TASC file name and data saving options. Use only with PARAM
CALC-METHOD=HETRAN/TASC-RIG or CALC-METHOD=AEROTRAN-RIG .

INPUT-FILE..... Name of Aspen Hetran/Aerotran (*.bjt) or HTFS TASC (*.tai) input file

SAV-HOT-STRM..... Whether to save Aspen Plus hot stream and curve data in the B-JAC or HTFS TASC input file.

SAV-HOT-STRM=YES	Save data in input file (Default)
SAV-HOT-STRM=NO	Do not save data in input file

SAV-CLD-STRM ..... Whether to save Aspen Plus cold stream and curve data in the B-JAC or HTFS TASC input file.

SAV-CLD-STRM=YES	Save data in input file (Default)
SAV-CLD-STRM=NO	Do not save data in input file

SAV-DSG-PARM..... Whether to save final geometry information from design in the B-JAC input file. This option is only available when using Hetran or Aerotran.

SAV-DSG-PARM=YES	Save data in input file (Default)
SAV-DSG-PARM=NO	Do not save data in input file

SAV-ANA-PARM ..... Whether to save Hetran parameters from the simulation in the B-JAC or HTFS TASC input file.

SAV-ANA-PARM=YES	Save data in input file (Default)
SAV-ANA-PARM=NO	Do not save data in input file

HOT-PCURVE, COLD-PCURVE

Use to set parameters to control the generation of property curves for the heat exchanger program specified in HETRAN-PARAM. Use only with PARAM CALC-METHOD=HETRAN-RIG or AEROTRAN-RIG.

GENERATE..... Determines which program generates property curves:

GENERATE=YES	Aspen Plus generates property curves using parameters supplied by the B-JAC or HTFS program. (Default)
GENERATE=-NO	Property curves are read from the B-JAC or HTFS input file.

UPDATE..... Controls how often Aspen Plus generates property curves:

UPDATE=ALWAYS	Calculates property curves at every block execution (Default)
UPDATE=NEVER	Calculates property curves only at the first block execution
UPDATE=AS-NEEDED	Calculates property curves if the range of the curve or the ends deviate by more than INDP-DEV from the previous execution

INDP-DEV ..... Controls the percent deviation Aspen Plus tolerates in the independent variable, before Aspen Plus recalculates the property curve

TYPE ..... Type of curve Aspen Plus generates

TYPE=ISOBARIC	Generate an isobaric property curve for B-JAC or HTFS program (Default)
TYPE=NON-ISOBARIC	Generate a non-isobaric property curve for B-JAC or HTFS program
TYPE=MULTI-ISOBAR	Generate three isobaric property curves for B-JAC or HTFS program

BJAC-INPUTS

Use to set B-JAC or HTFS input values. These values can be used in Aspen Plus simulation tools such as sensitivity, design-specs, and data fit.
Use only with PARAM CALC-METHOD=HETRAN-RIG or AEROTRAN-RIG .

HOT-FOULING..... Fouling factor for hot-side stream

HOT-FILM ..... Film coefficient for hot-side stream

HOT-PFACTOR..... Correction factor applied to the calculated hot-side pressure drop

HOT-FFACTOR..... Correction factor applied to the calculated hot-side film coefficient

HOT-MAX-DP..... Maximum allowable pressure drop to the hot-side stream

COLD-FOULING ..... Fouling factor for cold-side stream

COLD-FILM..... Film coefficient for cold-side stream

COLD-PFACTOR..... Correction factor applied to the calculated cold-side pressure drop

COLD-FFACTOR ..... Correction factor applied to the calculated cold-side film coefficient

COLD-MAX-DP..... Maximum allowable pressure drop to the cold-side stream

FOUL-OPTION..... Method for determining maximum fouling on each side (available to Hetran-rigorous method only)

FOUL-OPTION = PROGRAM	Adjust hot/cold-side fouling based on actual hot/cold fouling ratio (Default)
FOUL-OPTION = ADJ-HOT-COLD	Adjust hot/cold-side fouling based on specified fouling ratio
FOUL-OPTION = ADJ-HOT-ONLY	Adjust hot-side fouling only
FOUL-OPTION = ADJ-COLD-ONLY	Adjust cold-side fouling only

FOUL-RATIO..... Hot/cold-side fouling ratio. (Default = 1.0) (available to Hetran-rigorous method only)

PROPERTIES Use to override the global or flowsheet section property specifications. You can use different physical property option sets for the hot and cold sides of the heat exchanger. If you supply one set of property specifications, it will be used for both the hot-side and cold-side calculations. If you supply two sets, the first will be used for the hot-side, the second for the cold-side. Any option set name entered here must also be named in the PROPERTIES paragraph. (See Chapter 8.)

FLASH-SPECS Use to specify the flash options for the hot or cold-side of the heat exchanger. For each side of the heat exchanger, you can specify vapor phase, liquid phase, two-phase flash, or three-phase flash calculations.

sid..... Outlet stream ID. Flash specifications for the outlet stream will apply to all flash calculations on that side of the heat exchanger.

NPHASE..... Number of phases in MIXED substream:

NPHASE=1	One-phase calculation
NPHASE=2	Two-phase flash (Default)
NPHASE=3	Three-phase flash

PHASE..... Specifies the phase when NPHASE=1:

PHASE=V	Vapor (Default)
PHASE=L	Liquid
PHASE=S	Solid. Use for electrolytes system only.

FREE-WATER..... Use to override the free-water option established by the SIM-OPTIONS paragraph (see Chapter 45) or the BLOCK-OPTIONS sentence of the BLOCK paragraph (see Chapter 11).

FREE-WATER=NO	Does not perform free-water calculations
FREE-WATER=YES	Performs free-water calculations

MAXIT..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

TOL..... Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

HOT-HCURVE Use to generate cooling curve tables and plots for the hot-side of the heat exchanger. See Chapter 11 for a description of the input keywords.

COLD-HCURVE Use to generate heating curve tables and plots for the cold-side of the heat exchanger. See Chapter 11 for a description of the input keywords.

REPORT Use to override the default report options. You can use the standard REPORT options for use within a block (see Chapter 11) for HEATX.

reportopt..... Standard block report options (see Chapter 11) in addition to the following:

	PROFILE	Reports internal zone profiles

SUBROUTINE Use to specify user-supplied subroutines for calculating the heat transfer coefficient, LMTD correction factor, liquid holdup, and/or pressure drop on the tube side. See *Aspen Plus User Models*, Chapter 18, for a description on writing user-supplied subroutines for heat transfer coefficients and LMTD, and Chapter 17 for liquid holdup and pressure-drop subroutines.

HEAT-TR-COEF	Name of user-supplied FORTRAN subroutine for heat transfer coefficient calculations
LMTD-CORRECT	Name of user-supplied FORTRAN subroutine for log-mean temperature difference correction factor calculations
TUBE-DP-HLDP	Name of user-supplied FORTRAN subroutine to calculate liquid holdup in two-phase flow
TUBE-DP-PDRP	Name of user-supplied FORTRAN subroutine to calculate pressure-drop in two-phase flow

USER-VECS Use to define the length of arrays for user-supplied heat transfer coefficient, LMTD, and tube-side pressure-drop subroutines.

NINTU	Length of integer parameter array for the user-supplied heat transfer coefficient subroutine
NREALU	Length of real parameter array for the user-supplied heat transfer coefficient subroutine
NIWRKU	Length of integer workspace array for the user-supplied heat transfer coefficient subroutine
NWRKU	Length of real workspace array for the user-supplied heat transfer coefficient subroutine
NINTF	Length of integer parameter array for the user-supplied LMTD subroutine
NREALF	Length of real parameter array for the user-supplied pressure-drop subroutine
NIWRKF	Length of integer workspace array for the user-supplied LMTD subroutine
NWRKF	Length of real workspace array for the user-supplied LMTD subroutine
NINTH	Length of integer parameter array for the user-supplied liquid holdup subroutine
NREALH	Length of real parameter array for the user-supplied liquid holdup subroutine
NIWRKH	Length of integer workspace array for the user-supplied liquid holdup subroutine
NWRKH	Length of real workspace array for the user-supplied liquid holdup subroutine
NINTT	Length of integer parameter array for the user-supplied pressure-drop subroutine
NREALT	Length of real parameter array for the user-supplied pressure-drop subroutine
NIWRKT	Length of integer workspace array for the user-supplied pressure-drop subroutine

NWRKT ..... Length of real workspace array for the user-supplied pressure-drop subroutine

USER-INT-U Use to enter values for the integer parameter array of the user heat transfer coefficient subroutine.

value-list ..... List of integer values

USER-REAL-U Use to enter values for the real parameter array of the user heat transfer coefficient subroutine.

value-list ..... List of real values

USER-INT-F Use to enter values for the integer parameter array of the user LMTD correction factor subroutine.

value-list ..... List of integer values

USER-REAL-F Use to enter values for the real parameter array of the user LMTD correction factor subroutine.

value-list ..... List of real values

USER-INT-H Use to enter values for the integer parameter array of the user subroutine for tube-side liquid holdup.

value-list ..... List of integer values

USER-REAL-H Use to enter values for the real parameter array of the user subroutine for tube-side liquid holdup.

value-list ..... List of real values

USER-INT-T Use to enter values for the integer parameter array of the user subroutine for tube-side pressure drop.

value-list ..... List of integer values

USER-REAL-T Use to enter values for the real parameter array of the user subroutine for tube-side pressure drop.

value-list ..... List of real values

Table 13.1 Heat Exchanger Tube Materials

Keyword Value	Material†
CARBON-STEEL	Carbon Steel
C-H-MO-STEEL	C-1/2 Molybdenum Steel
1-CR-H-MO	1 Cr-1/2 Mo & 1-1/4 Cr-1/2 Mo
2-Q-CR-1-MO	2-1/4 Cr-1 Mo
5-CR-H-MO	5 Cr-1/2 Mo
7-CR-H-MO	7 Cr-1/2 Mo
9-CR-1-MO	9 Cr-1 Mo
3-H-NICKEL	3-1/2 Nickel
13-CR	13 Cr
15-CR	15 Cr
17-CR	17 Cr
TP-304-SS	TP 304 Stainless Steel
TP-316-SS	TP 316 Stainless Steel
TP-317-SS	TP 317 Stainless Steel
TP-321-SS	TP 321 Stainless Steel
TP-347-SS	TP 347 Stainless Steel
TP-310-SS	TP 310 Stainless Steel
NICKEL-200	Nickel 200
NI-CU-400	Ni-Cu Alloy 400
NI-CR-FE-600	Ni-Cr-Fe Alloy 600
NI-FE-CR-800	Ni-Fe-Cr Alloy 800
NI-FE-CR-MO-CU-825	Ni-Fe-Cr-Mo-Cu Alloy 825
NI-MO-B	Ni-Mo Alloy B
NI-MO-CR-C276	Ni-Mo-Cr Alloy C-276
ALUM-3003	Aluminum Alloy 3003
ALUM-6061	Aluminum Alloy 6061
TITANIUM	Titanium
ADMIRALTY	Admiralty Brass
NAVAL-BRASS	Naval Brass
COPPER	Copper
90-10-CU-NI	90-10 Copper/Nickel
70-30-CU-NI	70-30 Copper/Nickel

† HEATX uses standard construction materials defined in Standards of the Tubular Exchanger Manufacturers Association, Seventh Edition, 1988.

Accessing Variables in HEATX

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables
PARAM	T-HOT, T-COLD, DUTY, AREA, UA, DELT-HOT, DELT-COLD, DEGSUB-HOT, DEGSUP-COLD, VFRAC-HOT, VFRAC-COLD, DECR-HOT, INCR-COLD, LMTD-CORRECT, PRES-HOT, PRES-COLD, MIN-TAPP, MIN-OUT-TAPP
HEAT-TR-COEF	U, SCALE, REF-VALUE, EXPONENT, MOLE-RFLOW, MASS-RFLOW, STDVOL-RFLOW, L-L, B-L, V-L, L-B, B-B, V-B, L-V, B-V, V-V, UA
HOT-SIDE	H-SCALE, REF-VALUE, EXPONENT, MOLE-RFLOW, MASS-RFLOW, STDVOL-RFLOW, H, H-L, H-B, H-V, DP-SCALE, FOUL-FACTOR
COLD-SIDE	H-SCALE, REF-VALUE, EXPONENT, MASS-RFLOW, MOLE-RFLOW, STDVOL-RFLOW, H, H-L, H-B, H-V, DP-SCALE, FOUL-FACTOR
BJAC-INPUTS	HOT-FOULING, HOT-FILM, HOT-PFACTOR, HOT-FFACTOR, HOT-MAX-DP, COLD-FOULING, COLD-FILM, COLD-PFACTOR, COLD-FFACTOR, COLD-MAX-DP, FOUL-RATIO

Block Results

Description	Sentence	Variable	ID1 †
Exchanger heat duty	RESULTS	CALC-DUTY	—
Heat transfer area	RESULTS	CALC-AREA	—
Shell-side pressure drop	RESULTS	S-TOTAL-DP	—
Tube-side pressure drop	RESULTS	T-TOTAL-DP	—
Number of thermal transfer units	RESULTS	NTU	—
Heat transfer efficiency	RESULTS	XI	—
Log mean temperature difference correction factor	RESULTS	FMTD	—
Overall log mean temperature difference	RESULTS	DTLM	—
Overall area averaged dirty heat transfer coefficient	RESULTS	UAVD	—
Overall area averaged clean heat transfer coefficient	RESULTS	UAVC	—
Heat transfer mechanism for the section	SECT-REPORT	CONDITION	secno
Heat transfer for the section	SECT-REPORT	DUTY	secno
Area for the section	SECT-REPORT	AREA	secno
Hot stream temperature leaving the section	SECT-REPORT	THOT	secno
Cold stream temperature leaving the section	SECT-REPORT	TCOLD	secno
Log mean temperature difference for the section	SECT-REPORT	DTLM	secno
Area averaged heat transfer coefficient for the section	SECT-REPORT	UAVG	secno
UA	SECT-REPORT	UAV	secno
The side of the unit that has the hot stream	RESULTS	HOT-SIDE	—
Actual heat transfer area calculated from specified exchanger geometry	RESULTS	ACTUAL-AREA	—

† secno = section number.

continued

Block Results (continued)

Description	Sentence	Variable	ID1 †
Percentage of excess surface area available when unit is dirty	RESULTS	OVER-DESIGN	—
Percentage of excess surface area available when unit is clean	RESULTS	OVER-CLEAN	—
Number of shells in series (specified, or calculated in design mode)	RESULTS	NSHLS	—
Number of shells in parallel (specified)	RESULTS	NSHLP	—
Whether the unit has a potential vibration damage problem	RESULTS	VIB-IND	—
Whether the unit has an excess rho-v^2 problem	RESULTS	RHOV2-IND	—
UA	RESULTS	UA	
Number of flash points	FLS-PROFILE	NPOINT	—
Duty on hot side for a flash point	FLS-PROFILE	DUTY-HOT	ptno
Temperature on hot side for a flash point	FLS-PROFILE	T-HOT	ptno
Vapor fraction on hot side for a flash point	FLS-PROFILE	VF-HOT	ptno
Pressure on hot side for a flash point	FLS-PROFILE	P-HOT	ptno
Duty on cold side for a flash point	FLS-PROFILE	DUTY-COLD	ptno
Temperature on cold side for a flash point	FLS-PROFILE	T-COLD	ptno
Vapor fraction kn cold side for a flash point	FLS-PROFILE	VF-COLD	ptno
Pressure on cold side for a flash point	FLS-PROFILE	P-COLD	ptno
The number of the shell	EXCH-PROFILE	NEXCHS	exchno
Cumulative amount of heat transfer	EXCH-PROFILE	DUTY-CUM	exchno
Amount of heat transfer for the exchanger	EXCH-PROFILE	DUTY-INV	exchno
Overall heat transfer coefficient for the exchanger	EXCH-PROFILE	U-COEF	exchno
Area of the exchanger	EXCH-PROFILE	AREA	exchno
Log-mean temperature difference (uncorrected) for the exchanger	EXCH-PROFILE	LMTD	exchno
LMTD correction factor for the exchanger	EXCH-PROFILE	FT-FACTOR	exchno
Temperature of the hot stream at exchanger inlet	EXCH-PROFILE	T-HOT-IN	exchno
Temperature of the hot stream at exchanger outlet	EXCH-PROFILE	T-HOT-OT	exchno
Temperature of the cold stream at exchanger inlet	EXCH-PROFILE	T-CLD-IN	exchno
Temperature of the cold stream at exchanger outlet	EXCH-PROFILE	T-CLD-OT	exchno
Mass fraction of vapor of the hot stream at exchanger inlet	EXCH-PROFILE	VF-HOT-IN	exchno
Mass fraction of vapor of the hot stream at exchanger outlet	EXCH-PROFILE	VF-HOT-OT	exchno
Mass fraction of vapor of the cold stream at exchanger inlet	EXCH-PROFILE	VF-CLD-IN	exchno
Mass fraction of vapor of the cold stream at exchanger outlet	EXCH-PROFILE	VF-CLD-OT	exchno
Number of points from hot-side inlet to hot-side outlet	ZONE-PROFILE	NZONES	—

† ptno = point number; exchno = exchanger number.

continued

Block Results (continued)

Description	Sentence	Variable	ID1 †
The number of the shell	ZONE-PROFILE	EXCH-NO	zoneno
Total duty to this point	ZONE-PROFILE	DUTY-CUM	zoneno
Total duty for this shell to this point	ZONE-PROFILE	DUTY-EXC	zoneno
Duty for this interval	ZONE-PROFILE	DUTY	zoneno
Hot temperature at this point	ZONE-PROFILE	T-HOT	zoneno
Cold temperature at this point	ZONE-PROFILE	T-COLD	zoneno
Calculated area for this zone	ZONE-PROFILE	AREA	zoneno
Overall heat transfer coefficient for this interval	ZONE-PROFILE	U-COEF	zoneno
Corrected LMTD for this zone	ZONE-PROFILE	CMTD	zoneno
Temperature of the tube wall on the outside of the tube	SHELL-RESULT	WALL-TEMP	—
Average temperature of the fouling layer on the outside of the tube	SHELL-RESULT	SKIN-TEMP	—
Pressure drop for shell-side fluid flow without fouling. Includes pressure drop through all nozzles.	SHELL-RESULT	CLEAN-DP	—
Pressure drop for shell-side fluid flow with fouling present. Includes pressure drop through all nozzles.	SHELL-RESULT	DIRTY-DP	—
Pressure drop for shell-side fluide flow through baffle windows	SHELL-RESULT	WINDOW-DP	—
Pressure drop for shell-side fluid flow through the inlet and outlet zones of the exchanger	SHELL-RESULT	ENDS-DP	—
Pressure-drop for shell-side fluid flow across the bundle	SHELL-RESULT	CROSSFLOW-DP	—
Heat transfer coefficient between the bulk fluid and the fluid film on the heat transfer surface on the shell side of the exchanger	SHELL-RESULT	BULK-COEEF	—
Heat transfer coefficient at the tube wall on the shell side.	SHELL-RESULT	WALL-COEF	—
Overall thermal resistance on the outside of the tubes. (Inverse of overall heat transfer coefficient on the shell side.)	SHELL-RESULT	THERM-RESIST	—
Thermal resistance to heat transfer associated with the fouling layer on the outside of the tubes	SHELL-RESULT	FOUL-RESIST	—
Maximum amount of fouling on shell side under which exchanger can still meet specifications	SHELL-RESULT	MAX-FOUL-RESIST	—
Correction factor applied to shell-side heat transfer coefficient to reflect the presence of fins on tubes	SHELL-RESULT	FIN-CORR	—
Nominal velocity of the shell-side fluid that flows across the bundle	SHELL-RESULT	CROSSFLOW-VL	—
Nominal velocity of the shell-side fluid that flows through the baffle windows	SHELL-RESULT	WINDOW-VL	—
Velocity of fluid that flows across the bundle at a temperature point midway between the inlet and outlet temperatures of the exchanger	SHELL-RESULT	MIDPOINT-VL	—
The rho-v^2 (density x velocity^2) for the shell-side fluid as it enters the shell	SHELL-RESULT	SHL-IN-RHV2	—

† zoneno = zone number.

continued

Block Results (continued)

Description	Sentence	Variable	ID1
The rho-v^2 for the shell-side fluid as it exits the shell	SHELL-RESULT	SHL-OUT-RHV2	—
The rho-v^2 for the shell-side fluid as it enters the bundle	SHELL-RESULT	BND-IN-RHV2	—
The rho-v^2 for the shell-side fluid as it exits the bundle	SHELL-RESULT	BND-OUT-RHV2	—
Heat transfer efficiency of the additional surface area provided by external fins on the tubes	SHELL-RESULT	FIN-EFF	—
Percentage of overall thermal resistance to heat transfer associated with fouling on the outside of the tubes	SHELL-RESULT	FOUL-PERC	—
Percentage of overall resistance to heat transfer associated with shell-side resistance on the outside of the tubes	SHELL-RESULT	FILM-PERC	—
Temperature of the tube wall on the inside of the tube	TUBE-RESULT	WALL-TEMP	—
Average temperature of the fouling layer on the inside of the tube	TUBE-RESULT	SKIN-TEMP	—
Pressure drop for tube-side fluid flow without fouling. Includes pressure drop through all nozzles and tubes.	TUBE-RESULT	CLEAN-DP	—
Pressure drop for tube-side fluid flow with fouling present. Fouling layer reduces the flow area and increases the pressure drop. Includes pressure drop through all nozzles and tubes.	TUBE-RESULT	DIRTY-DP	—
Heat transfer coefficient between the bulk fluid and the fluid film on the heat transfer surface on the tube side of the exchanger	TUBE-RESULT	BULK-COEF	—
Heat transfer coefficient at the tube wall on the tube side.	TUBE-RESULT	WALL-COEF	—
Overall thermal resistance on the inside of the tubes. (Inverse of overall heat transfer coefficient on the tube side.)	TUBE-RESULT	THERM-RESIST	—
Thermal resistance to heat transfer associated with the fouling layer on the inside of the tubes	TUBE-RESULT	FOUL-RESIST	—
Maximum amount of fouling on tube side under which exchanger can still meet specifications	TUBE-RESULT	MAX-FOUL-RESIST	—
Velocity of the tube-side fluid as it enters the tubes immediately after entering the bundle	TUBE-RESULT	INLET-VL	—
Velocity of the tube-side fluid at a temperature point midway between the inlet and outlet temperatures of the exchanger	TUBE-RESULT	MIDPOINT-VL	—
Velocity of the tube-side fluid as it exits the tubes just prior to leaving the bundle	TUBE-RESULT	OUTLET-VL	—
Percentage of overall thermal resistance to heat transfer associated with fouling on the inside of the tubes	TUBE-RESULT	FOUL-PERC	—
Percentage of overall resistance to heat transfer associated with tube-side resistance on the inside of the tubes	TUBE-RESULT	FILM-PERC	—
Temperature of the tube wall on the outside of the tube	OUTSD-RESULT	WALL-TEMP	—

continued

Block Results (continued)

Description	Sentence	Variable	ID1
Average temperature of the fouling layer on the outside of the tube	OUTSD-RESULT	SKIN-TEMP	—
Flow rate of air across the outside surface of the tube bundle(s)	OUTSD-RESULT	AIR-FLOWRATE	—
Pressure drop of the flow of gas on the outside of the exchanger, assuming no fouling	OUTSD-RESULT	CLEAN-DP	—
Pressure drop of the flow of gas on the outside of the exchanger, on which a fouling layer exists	OUTSD-RESULT	DIRTY-DP	—
Pressure drop of the flow of gas across only the tube bundle	OUTSD-RESULT	BUNDLE-DP	—
Pressure drop of the flow of gas through the fan	OUTSD-RESULT	FAN-DP	—
Pressure drop of the flow of gas through the hail screen	OUTSD-RESULT	HAIL-SCR-DP	—
Pressure drop of the flow of gas through the fan guard	OUTSD-RESULT	FAN-GRD-DP	—
Pressure drop of the flow of gas through the stealm coil	OUTSD-RESULT	STM-COIL-DP	—
Pressure drop of the flow of gas through the louvre	OUTSD-RESULT	LOUVRE-DP	—
Pressure drop of the flow of gas to the exchanger, based on the exchanger's relative position to the ground and surrounding structures	OUTSD-RESULT	GROUND-DP	—
Heat-transfer coefficient between the bulk fluid and the fluid film on the heat-transfer surface on the outside of the tubes	OUTSD-RESULT	BULK-COEF	—
Overall thermal resistance to heat transfer on the outside of the tubes	OUTSD-RESULT	THERM-RESIST	—
Thermal resistance to heat transfer of the fouling layer on the outside of the tubes	OUTSD-RESULT	FOUL-RESIST	—
Thickness of the fouling layer on the outside of the tubes	OUTSD-RESULT	FOUL-THICK	—
Velocity of the gas stream at the inlet to the bundle	OUTSD-RESULT	BNDL-IN-VL	—
Velocity of the gas stream at the outlet of the bundle	OUTSD-RESULT	BNDL-OUT-VL	—
Velocity of the gas stream through the bundle, at a temperature midway between the inlet and outlet temperatures of the exchanger	OUTSD-RESULT	MIDPOINT-VL	—
Velocity of the gas stream immediately before it enters the bundle	OUTSD-RESULT	FACE-VL	—
Heat-transfer efficiency of the additional surface area provided by the external fins on the tubes	OUTSD-RESULT	FIN-EFF	—
Overall required brake power for the fans	FAN-RESULT	BRAKE-POWER	—
Fan blade tip speed required to generate the required gas flow rate and static pressure	FAN-RESULT	BLADE-SPEED	—
Noise level associated with the fans at a specific distance from the fan	FAN-RESULT	SOUND-PRES	—
Noise level associated with the operation of the fans	FAN-RESULT	SOUND-POWER	—
Overall power efficiency of the fans (the ratio of total air horsepower output to brake horsepower input)	FAN-RESULT	FAN-EFF	—

MHEATX: Multistream Heat Exchanger

Input Language for MHEATX

```
BLOCK    blockid    MHEATX
HOT-SIDE    keyword=value
COLD-SIDE    keyword=value
```

Keywords:

IN OUT

Optional keywords:

DECANT TEMP VFRAC DELT DEGSUP DEGSUB DUTY PRES NPHASE PHASE FREE-WATER MAXIT TOL Q-EST

```
PARAM    keyword=value
```

Optional keywords:

NPOINT MAXIT TOL T-UPPER T-LOWER TEST ADD-POINTS QLEAK QLEAK-FRAC ADAPTIVE-GRID DTTOL MAX-NPOINT FLOW-DIR DTCORR DTCORR2 TQTAB-NPOINT TQTAB-MAXNPT

```
STREAM-PROPERTIES    inlet-sid    opsetname    keyword=value  /  ...
```

Optional keywords:

FREE-WATER SOLU-WATER HENRY-COMPS

```
TQTAB-SPECS    inlet-sid    keyword=value  /  ...
```

Optional keywords:

NPOINT DPFRAC-VAP DPFRAC-2PH DPFRAC-LIQ

```
HCURVE    curveno    inlet-sid    keyword=value
```

Optional keywords:

INDEP-VAR LIST NPOINT INCR HEADING PROPERTIES PRES-PROFILE PDROP PRINT-PLOT HIGH-PRECISION LINES X-SCALE Y-SCALE WIDE GRID INTERPOLATE

```
REPORT    reportopt-list
```

Special reportopts:

NOPROFILE STREAMS NOTQTABLES

```
PLOT    plotno    plot-list    keyword=value
```

Plots:

TEMP DELT UA-DUTY TEMP-DELT DELT-TEMP UA-DELT UA-TEMP

Optional keywords:

Y-SCALE PLOT-HEADING WIDE GRID INTERPOLATE

Input Language Description for MHEATX

HOT-SIDE, COLD-SIDE

Use to enter inlet and outlet stream IDs, outlet specifications, and flash specifications for streams on the hot-side and cold-side of the exchanger, respectively. For each stream in the exchanger, you can specify vapor phase, liquid phase, two-phase flash, or three-phase flash calculations. You can also specify the outlet pressure or pressure drop for each stream in the exchanger.

IN	Inlet stream ID	
OUT	Outlet stream ID	
DECANT	Water decant stream ID	
TEMP	Outlet temperature	
VFRAC	Outlet vapor fraction	
DELT	Temperature change from the inlet	
DEGSUP	Degrees superheat at the outlet	
DEGSUB	Degrees subcooled at the outlet	
DUTY	Heat duty for the stream	
PRES	**PRES > 0**	Outlet pressure
	PRES ≤ 0	Pressure drop (Default=0)
Q-EST	An estimate of the enthalpy change of a stream in the heat exchanger. Use to set an initial value for the internal heat stream that goes from (internally generated) heater to (internally generated) mheater. Use when the internal heat stream is a tear stream. See Aspen Plus *Unit Operation Models*, Chapter 2, for information about the computational structure for MHEATX.	
NPHASE	Number of phases in MIXED substream:	
	NPHASE=1	One-phase calculation
	NPHASE=2	Two-phase flash (Default)
	NPHASE=3	Three-phase flash
PHASE	Specifies the phase when NPHASE=1:	
	PHASE=V	Vapor (Default)
	PHASE=L	Liquid
	PHASE=S	Solid. Use for electrolytes system only.
FREE-WATER	Use to override the free-water option established by the SIM-OPTIONS paragraph (see Chapter 45) or the BLOCK-OPTIONS sentence of the BLOCK paragraph (see Chapter 11).	
	FREE-WATER=NO	Does not perform free-water calculations
	FREE-WATER=YES	Performs free-water calculations
MAXIT	Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	
TOL	Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	

PARAM

Use to specify convergence parameters for the calculation to determine the temperature of unspecified streams. PARAM is also used to enter the number of zones for the internal analysis.

NPOINT	**NPOINT ≥ 1**	Number of zones for internal analysis
	NPOINT=0	Does not perform internal analysis (Default)

MAXIT ..... Maximum number of iterations to find outlet temperature of unspecified streams (Default=30)

TOL ..... Energy balance convergence tolerance, defined as a fraction of the heat transferred from the specified streams to the unspecified streams (Default=$1x10^{-4}$)

T-UPPER ..... Upper limit on temperature (Default=maximum of inlet temperatures + 1000K)

T-LOWER..... Lower limit on temperature (Default=100K, or minimum of inlet temperatures - 1000K, whichever is greater)

TEST ..... Initial temperature estimate

ADD POINTS ..... Specifies whether points should be added to the internal zone analysis for phase changes and stream additions:

ADD-POINTS=YES	Adds points to the zone analysis (Default)
ADD-POINTS=NO	Does not add points to the zone analysis

QLEAK..... Heat leak to or from the exchanger. A positive value for QLEAK represents transfer of heat into the exchanger. A negative value represents transfer of heat from the exchanger. (Default=0)

QLEAK-FRAC ..... Heat leak as a fraction of the heat transferred between the specified side of the exchanger and the unspecified side of the exchanger. (Default=0)

A positive value for QLEAK-FRAC represents transfer of heat from the surroundings into the exchanger. A negative value for QLEAK-FRAC represents transfer of heat from the exchanger to the surroundings.

If you specify the temperature of the hot-side:
QCOLD = QHOT (1 + QLEAK-FRAC)
If you specify the temperature of the cold-side:
QHOT = QCOLD (1 – QLEAK-FRAC)

ADAPTIVE-GRID ..... Specifies whether additional grid points will be inserted to account for the nonlinearity of the zone profile.

ADAPTIVE-GRID=YES	Adds grid points to zone analysis
ADAPTIVE-GRID=NO	Does not add grid points to zone analysis (Default)

DTTOL..... Threshold value of temperature approach above which additional points are inserted during ADAPTIVE-GRID calculation. You must also specify ADAPTIVE-GRID=YES and ADD-POINTS=YES.

MAX-NPOINT ..... Maximum number of points allowed in zone analysis. You must specify ADAPTIVE-GRID=YES and ADD-POINTS=YES.

FLOW-DIR..... Hot-side/cold-side flow direction. Use only in internal analysis.

FLOW-DIR=COCURRENT	Cocurrent flow
FLOW-DIR= COUNTERCURRENT	Countercurrent flow (Default)

DTCORR ..... Threshold value of temperature approach below which a penalty factor is applied to the calculated area

DTCORR2 ..... The penalty factor applied to the calculated area when temperature approach is less than DTCORR.

TQTAB-NPOINT..... Number of intervals used in generating T-Q tables

TQTAB-MAXNPT ..... Maximum number of intervals used when T-Q tables are generated for more than one stream. You must specify TQTAB-MAXNPT when you enter TQTAB-SPECS.

STREAM-PROPERTIES

Use to specify property options for an individual stream. You can use different physical property option sets for each stream in the exchanger. STREAM-PROPERTIES overrides the PROPERTIES sentence for an individual stream. The input language for STREAM-PROPERTIES is the same as for the PROPERTIES sentence (see Chapter 11), except that you must specify a stream ID for STREAM-PROPERTIES. Any option set name entered in a STREAM-PROPERTIES sentence must also be named in the PROPERTIES paragraph (see Chapter 8).

inlet-sid ..... Inlet stream ID

TQTAB-SPECS

Use to enter T-Q table specifications for internal zone analysis. When you specify a T-Q table for a stream, MHEATX generates a temperature enthalpy profile for that stream at the beginning of zone analysis calculations. During zone analysis, MHEATX interpolates the generated profile instead of performing stream flash calculations. This results in much faster execution times.

MHEATX assumes that pressure drop is proportional to duty during T-Q table generation and zone analysis. When you specify a T-Q table for a stream, you can also enter the fraction of total pressure drop (specified in HOT-SIDE or COLD-SIDE sentences) in each phase region.

When the fraction of pressure drop in a phase region is specified, MHEATX calculates the pressure drop for that region and generates a T-Q table. When generating the table, MHEATX assumes that pressure drop varies in proportion to duty in that region. You can enter up to two specifications from DPFRAC-VAP, DPFRAC-2PH, and DPFRAC-LIQ.

inlet-sid ..... Inlet stream ID

NPOINT..... Number of intervals used in generating the T-Q table for a stream. NPOINT overrides any value given for TQTAB-NPOINT in the PARAM sentence.

DPFRAC-VAP ..... Fraction of total pressure drop in the vapor region

DPFRAC-2PH ..... Fraction of total pressure drop in the two-phase region

DPFRAC-LIQ..... Fraction of total pressure drop in the liquid region

HCURVE

Use to generate heating or cooling curve tables and plots for a stream in the exchanger. See Chapter 11 for a description of the input keywords.

inlet-sid ..... Inlet stream ID

REPORT

Use to override the default report options. You can use the standard report options (see Chapter 11) for MHEATX.

reportopt ..... Standard block report options (see Chapter 11) in addition to the following:

NOPROFILE	Suppresses internal zone profiles
STREAMS	Generates stream profiles
NOTQTABLES	Does not report internally generated T-Q tables

PLOT

Use to create plots of internal profiles during an internal zone analysis.

plotno ..... Plot number

plot-list..... List of plots to be produced:

TEMP	Hot-side and cold-side temperature versus duty
DELT	Temperature difference versus duty
UA-DUTY	UA versus duty

	TEMP-DELT	Hot-side and cold-side temperature versus temperature difference
	DELT-TEMP	Temperature difference versus temperature
	UA-DELT	UA versus temperature difference
	UA-TEMP	UA versus temperature
Y-SCALE	**Y-SCALE=STANDARD**	Uses linear scale on vertical axis of plots (Default)
	Y-SCALE=LOG	Uses logarithmic scale on vertical axis of plots
PLOT-HEADING	Heading up to 64 characters enclosed in quotes, printed at the top of the print-plot	
WIDE, GRID, INTERPOLATE	Plot options. Use to override defaults established by PLOT-OPTIONS paragraph. (See Chapter 46.)	

Accessing Variables in MHEATX

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	ID2
HOT-SIDE	TEMP, VFRAC, DELT, DEGSUP, DEGSUB, DUTY, PRES, MAXIT, TOL	inlet-sid	—
COLD-SIDE	TEMP, VFRAC, DELT, DEGSUP, DEGSUB, DUTY, PRES, MAXIT, TOL	inlet-sid	—
HCURVE	NPOINT, INCR, PDROP	curveno	inlet-sid
PARAM	NPOINT, MAXIT, TOL, T-UPPER, T-LOWER, TEST	—	—

Block Results

Description	Sentence	Variable	ID1
Heat duty of a hot-side stream	HOT-SIDE	QCALC	inlet-sid
Heat duty of a cold-side stream	COLD-SIDE	QCALC	inlet-sid
Total UA	RESULTS	UA	—
Minimum internal temperature approach†	RESULTS	MITA	—
Average log mean temperature difference†	RESULTS	LMTD	—
Total exchanger duty†	RESULTS	DUTY	—
Cold-side temperature approach†	RESULTS	CSTA	—
Hot-side temperature approach†	RESULTS	HSTA	—
Heat duty	PROFILE	DUTY	pointno††
Hot-side temperature	PROFILE	THOT	pointno††
Cold-side temperature	PROFILE	TCOLD	pointno††
Temperature difference	PROFILE	DT†††	pointno††
Log mean temperature difference	PROFILE	LMTD	pointno††

† Calculated only when zone analysis is performed.

†† pointno is the sequential number of the zone.

continued

Block Results (continued)

Description	Sentence	Variable	ID1
UA	PROFILE	UA	pointno††
Base-temperature difference	BASE-PROFILE	DTBASE†††	pointno††

†† pointno is the sequential number of the zone.

††† You can also access variables using the VECTOR-DEF sentence. See Chapter 29.

HXFLUX: Heat Transfer Calculation

Input Language for HXFLUX

BLOCK **blockid** **HXFLUX**
PARAM *keyword=value*

Keywords:

THOT-IN TCOLD-IN HOT-IN COLD-IN

Optional keywords:

FLOW-DIR LMTD-METHOD THOT-OUT TCOLD-OUT HOT-OUT COLD-OUT DUTY DUTY-SID HEATSTRM-DIR U AREA MAXIT TOL

Input Language Description for HXFLUX

PARAM

Use to specify stream temperatures and heat transfer parameters. You must specify inlet hot stream temperature and inlet cold stream temperature, or their temperatures from referenced streams. You also need to specify three of outlet hot stream temperature, outlet cold stream temperature, overall heat transfer coefficient, and heat transfer area. If there is no inlet heat stream connected in the flowsheet, you also need to specify the duty or referenced heat stream.

THOT-IN ..... Inlet hot stream temperature

TCOLD-IN..... Inlet cold stream temperature

HOT-IN ..... Inlet hot stream ID

COLD-IN ..... Inlet cold stream ID

FLOW-DIR..... Flow direction in heat transfer calculation:

FLOW-DIR= COUNTERCURRENT	Countercurrent heat transfer (Default)
FLOW-DIR=COCURRENT	Cocurrent heat transfer

LMTD-METHOD..... Calculation method for log-mean temperature difference (See note 1.):

LMTD-METHOD=RIGOROUS	Rigorous method (Default)
LMTD-METHOD= APPROXIMATE	Approximate method

THOT-OUT..... Outlet hot stream temperature

TCOLD-OUT ..... Outlet cold stream temperature

HOT-OUT ..... Outlet hot stream ID

COLD-OUT ..... Outlet cold stream ID

DUTY ..... Heat duty

DUTY-SID ..... Heat stream ID

HEATSTRM-DIR ..... Heat stream direction

HEATSTRM-DIR= HOT-TO-COLD	Heat stream is from hot side to cold side (with a positive duty value)
HEATSTRM-DIR= COLD-TO-HOT	Heat stream is from cold side to hot side (with a negative duty value)

U ..... Overall heat transfer coefficient

AREA ..... Heat transfer area

MAXIT ..... Maximum number of iterations (Default=20)

TOL ..... Convergence tolerance (Default=1.D-4)

Accessing Variables in HXFLUX

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables
PARAM	THOT-IN, TCOLD-IN, THOT-OUT, TCOLD-OUT, DUTY, U, AREA

Block Results

Description	Sentence	Variable
Inlet hot stream temperature	RESULTS	THOT-INLET
Inlet cold stream temperature	RESULTS	TCOLD-INLET
Outlet hot stream temperature	RESULTS	THOT-OUTLET
Outlet cold stream temperature	RESULTS	TCOLD-OUTLET
Log-mean temperature difference	RESULTS	LMTD
Overall heat transfer coefficient	RESULTS	UCALC
Heat transfer area	RESULTS	AREA-CALC
Heat duty used	RESULTS	QCALC

Note

1 For convective heat transfer, the model equation is:

$$Q = U \times A \times LMTD$$

If the rigorous method is used,

$$LMTD = \frac{\Delta T_1 - \Delta T_2}{\ln\left(\frac{\Delta T_1}{\Delta T_2}\right)}.$$

If the approximate method is used,

$$LMTD = \left(\frac{\Delta T_1^{1/3} + \Delta T_2^{1/3}}{2}\right)^3.$$

Where:

A	=	Heat transfer area
$\Delta T_1, \Delta T_2$	=	Approach temperatures
$LMTD$	=	Log-mean temperature difference
Q	=	Heat duty
U	=	Overall heat transfer coefficient

HETRAN: Interface to the B-JAC HETRAN Program for Shell and Tube Heat Exchangers

Input Language for HETRAN

BLOCK **blockid** **HETRAN**
PARAM *keyword=value*

Keywords:

INPUT-FILE **CALC-TYPE** **T-HOT** **T-COLD** **DUTY** **DELT-HOT** **DELT-COLD** **DEGSUB-HOT** **DEGSUP-COLD** **VFRAC-HOT** **VFRAC-COLD** **DECR-HOT** **INCR-COLD**

Optional keywords:

SAV-HOT-STRM **SAV-CLD-STRM** **SAV-DSG-PARM** **SAV-ANA-PARM**

FEEDS **HOT=***sid* **COLD=***sid*
PRODUCTS **HOT=***sid* **COLD=***sid*
DECANT-STREAMS **[HOT=***sid***]** **[COLD=***sid***]**
HOT-PCURVE *keyword=value*

Optional keywords:

GENERATE **UPDATE** **INDP-DEV** **TYPE**

COLD-PCURVE *keyword=value*

Optional keywords:

GENERATE **UPDATE** **INDP-DEV** **TYPE**

BJAC-INPUTS *keyword=value*

Optional keywords:

HOT-FOULING **HOT-FILM** **HOT-PFACTOR** **HOT-FFACTOR** **HOT-MAX-DP** **COLD-FOULING** **COLD-FILM** **COLD-PFACTOR** **COLD-FFACTOR** **COLD-MAX-DP** **FOUL-OPTION** **FOUL-RATIO**

PROPERTIES *opsetname* *keyword=value* **[/** *opsetname* *keyword=value***]**

Optional keywords:

FREE-WATER **SOLU-WATER** **HENRY-COMPS**

FLASH-SPECS *sid* *keyword=value*

Optional keywords:

NPHASE **PHASE** **FREE-WATER** **MAXIT** **TOL**

Input Language Description for HETRAN

PARAM

Use to enter overall parameters for the block.

INPUT-FILE ..... Name of the B-JAC heat exchanger program input file

CALC-TYPE ..... Type of heat exchanger calculation.

CALC-TYPE = DESIGN	Select the geometry based on process conditions
CALC-TYPE = RATING	Determine if exchanger is over or under-surfaced based on the given geometry
CALC-TYPE = SIMULATION	Determine outlet conditions assuming surface area is fully utilized

T-HOT ..... Outlet temperature of the hot stream

T-COLD ..... Outlet temperature of the cold stream

DUTY..... Exchanger heat duty

DELT-HOT ..... Temperature approach at the hot stream outlet

DELT-COLD ..... Temperature approach at the cold stream outlet

DEGSUB-HOT ..... Degrees of subcooling of hot stream outlet

DEGSUP-COLD..... Degrees of superheat of cold stream outlet

VFRAC-HOT..... Vapor fraction of hot stream outlet

VFRAC-COLD ..... Vapor fraction of cold stream outlet

DECR-HOT..... Temperature decrease of the hot stream

INCR-COLD ..... Temperature increase of the cold stream

SAV-HOT-STRM..... Determines whether to save Aspen Plus hot-stream data in the B-JAC input file:

SAV-HOT-STRM=YES	Writes Aspen Plus hot-stream data to the B-JAC input file at the end of the simulation (Default)
SAV-HOT-STRM=NO	Does not write Aspen Plus hot-stream data to the B-JAC input file

SAV-CLD-STRM ..... Determines whether to save Aspen Plus cold-stream data in the B-JAC input file:

SAV-CLD-STRM=YES	Writes Aspen Plus cold-stream data to the B-JAC input file at the end of the simulation (Default)
SAV-CLD-STRM=NO	Does not write Aspen Plus cold-stream data to the B-JAC input file

SAV-DSG-PARM..... Whether to save final geometry information from design in the B-JAC input file.

SAV-DSG-PARM=YES	Save data in B-JAC input file (Default)
SAV-DSG-PARM=NO	Do not save data in B-JAC input file

SAV-ANA-PARM ..... Whether to save Hetran parameters from the simulation in the B-JAC input file.

SAV-ANA-PARM=YES	Save data in B-JAC input file (default)
SAV-ANA-PARM=NO	Do not save data in B-JAC input file

FEEDS, PRODUCTS, DECANT_STREAMS

Use to identify inlet and outlet streams. You must identify hot and cold inlets and outlets, and any water decant streams.

HOT-SIDE ..... Stream ID for the hot side

COLD-SIDE..... Stream ID for the cold side

HOT-PCURVE, COLD-PCURVE

Use to set parameters to control the generation of property curves for the B-JAC heat exchanger program HETRAN.

GENERATE..... Determines which program generates property curves:

GENERATE=YES	Aspen Plus generates property curves using parameters supplied by the B-JAC program. (Default)
GENERATE=-NO	Property curves are read from the B-JAC input file.

UPDATE..... Controls how often Aspen Plus generates property curves:

UPDATE=ALWAYS	Calculates property curves at every block execution (Default)
UPDATE=NEVER	Calculates property curves only at the first block execution
UPDATE=AS-NEEDED	Calculates property curves if the range of the curve or the ends deviate by more than INDP-DEV from the previous execution

INDP-DEV ..... Controls the percent deviation Aspen Plus tolerates in the independent variable, before Aspen Plus recalculates the property curve

TYPE ..... Type of curve Aspen Plus generates

TYPE=ISOBARIC	Generate an isobaric property curve for Hetran program (Default)
TYPE=NON-ISOBARIC	Generate a non-isobaric property curve for Hetran program

BJAC-INPUTS

Use to set B-JAC input values. These values can be used in Aspen Plus simulation tools such as sensitivity, design-specs, and datafit.

HOT-FOULING..... Fouling factor for hot-side stream

HOT-FILM ..... Film coefficient for hot-side stream

HOT-PFACTOR..... Correction factor applied to the calculated hot-side pressure drop

HOT-FFACTOR..... Correction factor applied to the calculated hot-side film coefficient

HOT-MAX-DP..... Maximum allowable pressure drop to the hot-side stream

COLD-FOULING..... Fouling factor for cold-side stream

COLD-FILM..... Film coefficient for cold-side stream

COLD-PFACTOR..... Correction factor applied to the calculated cold-side pressure drop

COLD-FFACTOR..... Correction factor applied to the calculated cold-side film coefficient

COLD-MAX-DP..... Maximum allowable pressure drop to the cold-side stream

FOUL-OPTION..... Method for determining maximum fouling on each side

FOUL-OPTION = PROGRAM	Adjust hot/cold-side fouling based on actual hot/cold fouling ratio (Default)
FOUL-OPTION = ADJ-HOT-COLD	Adjust hot/cold-side fouling based on specified fouling ratio
FOUL-OPTION = ADJ-HOT-ONLY	Adjust hot-side fouling only
FOUL-OPTION = ADJ-COLD-ONLY	Adjust cold-side fouling only

FOUL-RATIO ..... Hot/cold-side fouling ratio. (Default = 1.0)

PROPERTIES Use to override global or flowsheet section property specifications. You can use different physical property option sets for the hot and cold sides of the exchanger. If you supply one set of property specifications, Aspen Plus uses the set for both hot-side and cold-side calculations. If you supply two sets, Aspen Plus uses the first set for the hot side, and the second set for the cold side. If you enter an option set name, you must also enter the name in the PROPERTIES paragraph. (See Chapter 8.)

FLASH-SPECS Use to specify flash options for the hot or cold side of the heat exchanger. For each side of the heat exchanger, you can specify vapor phase, liquid phase, two-phase flash, or three-phase flash calculations.

sid..... Outlet stream ID. Flash specifications for the outlet stream apply to all flash calculations on that side of the heat exchanger.

NPHASE ..... Number of phases in MIXED substream:

NPHASE=1	One-phase calculation
NPHASE=2	Two-phase flash (Default)
NPHASE=3	Three-phase flash

PHASE..... Specifies the phase when NPHASE=1

PHASE=V	Vapor (Default)
PHASE=L	Liquid
PHASE=S	Solid. Use for electrolytes system only.

FREE-WATER..... Use to override the free-water option established by the SIM-OPTIONS paragraph. (See Chapter 45.) Or use to override the free-water option established by the BLOCK-OPTIONS sentence of the BLOCK paragraph. (See Chapter 11.)

FREE-WATER=NO	Does not perform free-water calculations
FREE-WATER=YES	Performs free-water calculations

MAXIT..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph. See Chapter 45.)

TOL..... Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph. See chapter 45.)

Accessing Variables in HETRAN

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables
BJAC-INPUTS	HOT-FOULING, HOT-FILM, HOT-PFACTOR, HOT-FFACTOR, HOT-MAX-DP, COLD-FOULING, COLD-FILM, COLD-PFACTOR, COLD-FFACTOR, COLD-MAX-DP, FOUL-RATIO

Block Results

Description	Sentence	Variable
Total heat load transferred between the process streams in the heat exchanger	UNIT-RESULT	HEAT-DUTY
Total outside surface area of all tubes in the heat exchanger	UNIT-RESULT	TOTAL-AREA
Overall rate at which heat is transferred from the hot fluid to the cold fluid	UNIT-RESULT	OVERALL-COEF
Effective temperature difference for the entire exchanger	UNIT-RESULT	EFF-DELTA-T
Correction factor applied to the log-mean temperature difference, to correct for flow arrangements that are not true counter-current	UNIT-RESULT	LMTD-CORRECT
The side of the unit that has the hot stream	UNIT-RESULT	HOT-SIDE
Whether the unit has a potential vibration damage problem	UNIT-RESULT	VIB-IND
Whether the unit has an excess rho-v^2 problem	UNIT-RESULT	RHOV2-IND
Percentage of excess surface area available when unit is dirty	UNIT-RESULT	OVER-DESIGN
Percentage of excess surface area available when unit is clean	UNIT-RESULT	OVER-CLEAN
Calculated average heat transfer coefficient for the entire exchanger in clean service (with fouling factors set to zero)	UNIT-RESULT	AVG-U-CLEAN
Calculated average heat transfer coefficient for the entire exchanger in dirty service (using fouling factors)	UNIT-RESULT	OVERALL-COEF
Area required to transfer the heat load	UNIT-RESULT	CALC-AREA
Actual physical exchanger area	UNIT-RESULT	TOTAL-AREA
Temperature of the tube wall on the outside of the tubes	SHELL-RESULT	WALL-TEMP
Average temperature of the fouling layer on the outer surface of the tubes	SHELL-RESULT	SKIN-TEMP
Pressure drop of the fluid flow on the shell side of the exchanger, without fouling	SHELL-RESULT	CLEAN-DP

continued

Block Results (continued)

Description	Sentence	Variable
Pressure drop of the fluid flow on the shell side of the exchanger, with fouling present	SHELL-RESULT	DIRTY-DP
Pressure drop of the shell-side fluid flow through the baffle windows	SHELL-RESULT	WINDOW-DP
Pressure drop of the shell-side fluid flow through the inlet and outlet zones of the exchanger	SHELL-RESULT	ENDS-DP
Pressure drop of the flow of the shell-side fluid across the bundle	SHELL-RESULT	CROSSFLOW-DP
Heat-transfer coefficient between the bulk fluid and the fluid film on the heat-transfer surface, for the shell side of the exchanger	SHELL-RESULT	BULK-COEF
Heat-transfer coefficient at the tube wall, for the shell side of the exchanger	SHELL-RESULT	WALL-COEF
Overall thermal resistance to heat transfer on the outside of the tubes	SHELL-RESULT	THERM-RESIST
Thermal resistance to heat transfer of the fouling layer on the outside of the tubes	SHELL-RESULT	FOUL-RESIST
Maximum amount of fouling on shell side under which exchanger can still meet specifications	SHELL-RESULT	MAX-FOUL-RESIST
Correction factor applied to the shell-side heat-transfer coefficient, to reflect the presence of fins on the tubes	SHELL-RESULT	FIN-CORR
Correction factor applied to the log-mean temperature difference, to account for thermal leakage across the longitudinal baffle on the shell side of the exchanger	SHELL-RESULT	LBAF-CORR
Nominal velocity of that portion of the shell-side fluid that flows across the bundle	SHELL-RESULT	CROSSFLOW-VL
Nominal velocity of the shell-side fluid that flows through the baffle windows	SHELL-RESULT	WINDOW-VL
Velocity of the shell-side fluid that flows across the bundle, at a temperature midway between the inlet and outlet temperatures of the exchanger	SHELL-RESULT	MIDPOINT-VL
rho-v^2 (density x velocity^2) for the shell-side fluid, as it enters the shell	SHELL-RESULT	SHL-IN-RHV2
rho-v^2 for the shell-side fluid, as it exits the shell	SHELL-RESULT	SHL-OUT-RHV2
rho-v^2 for the shell-side fluid, as it enters the bundle	SHELL-RESULT	BND-IN-RHV2
rho-v^2 for the shell-side fluid, as it exits the bundle	SHELL-RESULT	BND-OUT-RHV2
Heat-transfer efficiency of the additional surface area provided by the external fins on the tubes	SHELL-RESULT	FIN-EFF
Percentage of overall thermal resistance to heat transfer associated with fouling on the outside of the tubes	SHELL-RESULT	FOUL-PERC
Percentage of overall resistance to heat transfer associated with shell-side resistance on the outside of the tubes	SHELL-RESULT	FILM-PERC
Temperature of the tube wall on the inside of the tubes	TUBE-RESULT	WALL-TEMP
Temperature of the fouling layer on the inside of the tubes	TUBE-RESULT	SKIN-TEMP

continued

Block Results (continued)

Description	Sentence	Variable
Pressure drop of the fluid on the inside of the tubes, assuming no fouling is present	TUBE-RESULT	CLEAN-DP
Pressure drop of the fluid on the inside of the tubes, assuming fouling is present	TUBE-RESULT	DIRTY-DP
Heat-transfer coefficient between the bulk fluid and the fluid film, for the tube side of the exchanger	TUBE-RESULT	BULK-COEF
Heat-transfer coefficient at the tube wall on the tube side of the exchanger	TUBE-RESULT	WALL-COEF
Thermal resistance to heat transfer for the tube-side fluid	TUBE-RESULT	THERM-RESIST
Thermal resistance to heat transfer due to fouling on the tube side of the exchanger	TUBE-RESULT	FOUL-RESIST
Maximum amount of fouling on tube side under which exchanger can still meet specifications	TUBE-RESULT	MAX-FOUL-RESIST
Thickness of fouling layer on the tube side of the exchanger	TUBE-RESULT	FOUL-THICK
Velocity of the tube-side fluid as it enters the tubes, immediately after entering the bundle	TUBE-RESULT	INLET-VL
Velocity of the tube-side fluid as it exits the tubes, prior to leaving the bundle	TUBE-RESULT	OUTLET-VL
Velocity of the tube-side fluid, at a temperature midway between the inlet and outlet temperatures of the exchanger	TUBE-RESULT	MIDPOINT-VL
Percentage of overall thermal resistance to heat transfer associated with fouling on the inside of the tubes	TUBE-RESULT	FOUL-PERC
Percentage of overall resistance to heat transfer associated with tube-side resistance on the inside of the tubes	TUBE-RESULT	FILM-PERC

AEROTRAN: Interface to the B-JAC AEROTRAN Program for Air Cooled Heat Exchangers

Input Language for AEROTRAN

BLOCK **blockid** **AEROTRAN**
PARAM *keyword=value*

Keywords:

INPUT-FILE

Optional keywords:

CREATE-FILE **BJAC-UNITS** **SAV-HOT-STRM** **SAV-CLD-STRM**

FEEDS **HOT=***sid* **COLD=***sid*
PRODUCTS **HOT=***sid* **COLD=***sid*
DECANT-STREAMS **[HOT=***sid***]** **[COLD=***sid***]**

HOT-PCURVE *keyword=value*

Optional keywords:

GENERATE UPDATE SAVE-CURVE INDP-DEV TYPE

COLD-PCURVE *keyword=value*

Optional keywords:

GENERATE UPDATE SAVE-CURVE INDP-DEV TYPE

BJAC-INPUTS *keyword=value*

Optional keywords:

HOT-FOULING HOT-FILM HOT-PFACTOR
COLD-FOULING COLD-FILM COLD-PFACTOR

PROPERTIES *opsetname keyword=value* [**/** *opsetname keyword=value*]

Optional keywords:

FREE-WATER SOLU-WATER HENRY-COMPS

FLASH-SPECS *sid keyword=value*

Optional keywords:

NPHASE PHASE FREE-WATER MAXIT TOL

Input Language Description for AEROTRAN

PARAM

Use to enter overall parameters for the block.

INPUT-FILE..... Name of the B-JAC heat exchanger program input file

CREATE-FILE..... Determines whether to create the B-JAC input file, if it does not currently exist:

CREATE-FILE=NO	Does not create the B-JAC input file.
CREATE-FILE=YES	Creates the B-JAC input file at the end of the simulation, if the file does not exist

BJAC-UNITS..... Determines which B-JAC unit set will be used when creating a new input file:

BJAC-UNITS=US	Uses B-JAC US engineering units
BJAC-UNITS=SI	Uses B-JAC SI units
BJAC-UNITS=METRIC	Uses B-JAC metric units

SAV-HOT-STRM..... Determines whether to save Aspen Plus hot-stream data in the B-JAC input file:

SAV-HOT-STRM=NO	Does not write Aspen Plus hot-stream data to the B-JAC input file (Default)
SAV-HOT-STRM=YES	Writes Aspen Plus hot-stream data to the B-JAC input file, at the end of the simulation

SAV-CLD-STRM ..... Determines whether to save Aspen Plus cold-stream data in the B-JAC input file:

SAV-CLD-STRM=NO	Does not write Aspen Plus cold-stream data to the B-JAC input file (Default)
SAV-CLD-STRM=YES	Writes Aspen Plus cold-stream data to the B-JAC input file, at the end of the simulation

FEEDS, PRODUCTS, DECANT_STREAMS

Use to identify inlet and outlet streams. You must identify hot and cold inlets and outlets, and any water decant streams.

HOT-SIDE ..... Stream ID for the hot side

COLD-SIDE..... Stream ID for the cold side

HOT-PCURVE, COLD-PCURVE

Use to set parameters to control the generation of property curves for the B-JAC heat exchanger program AEROTRAN.

GENERATE..... Determines which program generates property curves:

GENERATE=YES	Aspen Plus generates property curves using parameters supplied by the B-JAC program. (Default)
GENERATE=-NO	Property curves are read from the B-JAC input file.

UPDATE..... Controls how often Aspen Plus generates property curves:

UPDATE=ALWAYS	Calculates property curves at every block execution (Default)
UPDATE=NEVER	Calculates property curves only at the first block execution
UPDATE=AS-NEEDED	Calculates property curves if the range of the curve or the ends deviate by more than INDP-DEV from the previous execution

SAVE-CURVE ..... Determines whether to save the Aspen Plus property curve in the B-JAC input file:

SAVE-CURVE=NO	Does not write the property curve to the B-JAC input file (Default)
SAVE-CURVE=YES	Writes the property curve to the B-JAC input file, at the end of the simulation

INDP-DEV ..... Controls the percent deviation Aspen Plus tolerates in the independent variable, before Aspen Plus recalculates the property curve

TYPE ..... Type of curve Aspen Plus generates

TYPE=ISOBARIC	Generate an isobaric property curve for Aerotran program (Default)
TYPE=NON-ISOBARIC	Generate a non-isobaric property curve for Aerotran program

BJAC-INPUTS

Use to set B-JAC input values. These values can be used in Aspen Plus simulation tools such as sensitivity, design-specs, and datafit.

HOT-FOULING..... Fouling factor for the hot-side stream

HOT-FILM ..... Film coefficient for the hot-side stream

HOT-PFACTOR..... Correction factor applied to the calculated hot-side pressure drop

COLD-FOULING..... Fouling factor for the cold-side stream

COLD-FILM..... Film coefficient for the cold-side stream

COLD-PFACTOR..... Correction factor applied to the calculated cold-side pressure drop

PROPERTIES

Use to override global or flowsheet section property specifications. You can use different physical property option sets for the hot and cold sides of the exchanger. If you supply one set of property specifications, Aspen Plus uses the set for both hot-side and cold-side calculations. If you supply two sets, Aspen Plus uses the first set for the hot side, and the second set for the cold side. If you enter an option set name, you must also enter the name in the PROPERTIES paragraph. (See Chapter 8.)

FLASH-SPECS

Use to specify flash options for the hot or cold side of the heat exchanger. For each side of the heat exchanger, you can specify vapor phase, liquid phase, two-phase flash, or three-phase flash calculations.

sid..... Outlet stream ID. Flash specifications for the outlet stream apply to all flash calculations on that side of the heat exchanger.

NPHASE ..... Number of phases in MIXED substream:

NPHASE=1	One-phase calculation
NPHASE=2	Two-phase flash (Default)
NPHASE=3	Three-phase flash

PHASE..... Specifies the phase when NPHASE=1

PHASE=V	Vapor (Default)
PHASE=L	Liquid
PHASE=S	Solid. Use for electrolytes system only.

FREE-WATER..... Use to override the free-water option established by the SIM-OPTIONS paragraph. (See Chapter 45.) Or use to override the free-water option established by the BLOCK-OPTIONS sentence of the BLOCK paragraph. (See Chapter 11.)

FREE-WATER=NO	Does not perform free-water calculations
FREE-WATER=YES	Performs free-water calculations

MAXIT..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph. See Chapter 45.)

TOL ..... Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph. See chapter 45.)

Accessing Variables in AEROTRAN

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables
BJAC-INPUTS	HOT-FOULING, HOT-FILM, HOT-PFACTOR, COLD-FOULING, COLD-FILM, COLD-PFACTOR

Block Results

Description	Sentence	Variable
Total heat load transferred between the process streams in the heat exchanger	UNIT-RESULT	HEAT-DUTY
Total outside surface area of all tubes in the heat exchanger	UNIT-RESULT	TOTAL-AREA
Total outside surface area of the tubes that is available for heat transfer	UNIT-RESULT	EFFECT-AREA
Overall rate at which heat is transferred from the hot fluid to the cold fluid	UNIT-RESULT	OVERALL-COEF
Effective temperature difference for the entire exchanger	UNIT-RESULT	EFF-DELTA-T

continued

Block Results (continued)

Description	Sentence	Variable
Correction factor applied to the log-mean temperature difference, to correct for flow arrangements that are not true counter-current	UNIT-RESULT	LMTD-CORRECT
Temperature of the tube wall on the outside of the tubes	OUTSD-RESULT	WALL-TEMP
Average temperature of the fouling layer on the outer surface of the tubes	OUTSD-RESULT	SKIN-TEMP
Flow rate of air across the outside surface of the tube bundle(s)	OUTSD-RESULT	AIR-FLOWRATE
Pressure drop of the flow of gas on the outside of the exchanger, assuming no fouling	OUTSD-RESULT	CLEAN-DP
Pressure drop of the flow of gas on the outside of the exchanger, on which a fouling layer exists	OUTSD-RESULT	DIRTY-DP
Pressure drop of the flow of gas across only the tube bundle	OUTSD-RESULT	BUNDLE-DP
Pressure drop of the flow of gas through the fan	OUTSD-RESULT	FAN-DP
Pressure drop of the flow of gas through the hail screen	OUTSD-RESULT	HAIL-SCR-DP
Pressure drop of the flow of gas through the fan guard	OUTSD-RESULT	FAN-GRD-DP
Pressure drop of the flow of gas through the stealm coil	OUTSD-RESULT	STM-COIL-DP
Pressure drop of the flow of gas through the louvre	OUTSD-RESULT	LOUVRE-DP
Pressure drop of the flow of gas to the exchanger, based on the exchanger's relative position to the ground and surrounding structures	OUTSD-RESULT	GROUND-DP
Heat-transfer coefficient between the bulk fluid and the fluid film on the heat-transfer surface on the outside of the tubes	OUTSD-RESULT	BULK-COEF
Overall thermal resistance to heat transfer on the outside of the tubes	OUTSD-RESULT	THERM-RESIST
Thermal resistance to heat transfer of the fouling layer on the outside of the tubes	OUTSD-RESULT	FOUL-RESIST
Thickness of the fouling layer on the outside of the tubes	OUTSD-RESULT	FOUL-THICK
Velocity of the gas stream at the inlet to the bundle	OUTSD-RESULT	BNDL-IN-VL
Velocity of the gas stream at the outlet of the bundle	OUTSD-RESULT	BNDL-OUT-VL
Velocity of the gas stream through the bundle, at a temperature midway between the inlet and outlet temperatures of the exchanger	OUTSD-RESULT	MIDPOINT-VL
Velocity of the gas stream immediately before it enters the bundle	OUTSD-RESULT	FACE-VL
Heat-transfer efficiency of the additional surface area provided by the external fins on the tubes	OUTSD-RESULT	FIN-EFF
Temperature of the tube wall on the inside of the tubes	TUBE-RESULT	WALL-TEMP
Temperature of the fouling layer on the inside of the tubes	TUBE-RESULT	SKIN-TEMP
Pressure drop of the fluid on the inside of the tubes, assuming no fouling is present	TUBE-RESULT	CLEAN-DP

continued

Block Results (continued)

Description	Sentence	Variable
Pressure drop of the fluid on the inside of the tubes, assuming fouling is present	TUBE-RESULT	DIRTY-DP
Heat-transfer coefficient between the bulk fluid and the fluid film, for the tube side of the exchanger	TUBE-RESULT	BULK-COEF
Heat-transfer coefficient at the tube wall on the tube side of the exchanger	TUBE-RESULT	WALL-COEF
Thermal resistance to heat transfer for the tube-side fluid	TUBE-RESULT	THERM-RESIST
Thermal resistance to heat transfer due to fouling on the tube side of the exchanger	TUBE-RESULT	FOUL-RESIST
Thickness of fouling layer on the tube side of the exchanger	TUBE-RESULT	FOUL-THICK
Velocity of the tube-side fluid as it enters the tubes, immediately after entering the bundle	TUBE-RESULT	INLET-VL
Velocity of the tube-side fluid as it exits the tubes, prior to leaving the bundle	TUBE-RESULT	OUTLET-VL
Velocity of the tube-side fluid, at a temperature midway between the inlet and outlet temperatures of the exchanger	TUBE-RESULT	MIDPOINT-VL
Overall required brake power for the fans	FAN-RESULT	BRAKE-POWER
Fan blade tip speed required to generate the required gas flow rate and static pressure	FAN-RESULT	BLADE-SPEED
Noise level associated with the fans at a specific distance from the fan	FAN-RESULT	SOUND-PRES
Noise level associated with the operation of the fans	FAN-RESULT	SOUND-POWER
Overall power efficiency of the fans (the ratio of total air horsepower output to brake horsepower input)	FAN-RESULT	FAN-EFF

HTRIXIST: Interface to the HTRI XIST Program for Shell and Tube Heat Exchangers

Input Language for HTRIXIST

```
BLOCK    blockid    HTRIXIST
PARAM    keyword=value
```

Keywords:

INPUT-FILE

Optional keywords:

CREATE-FILE HTRI-UNITS SAV-HOT-STRM SAV-CLD-STRM

```
FEEDS    HOT=sid    COLD=sid
PRODUCTS    HOT=sid    COLD=sid
DECANT-STREAMS    [HOT=sid]    [COLD=sid]
HOT-PCURVE
```

Optional keywords:

GENERATE UPDATE SAVE-CURVE INDP-DEV

```
COLD-PCURVE
```

Optional keywords:

GENERATE UPDATE SAVE-CURVE INDP-DEV

```
HTRI-INPUTS
```

Optional keywords:

HOT-FOULING HOT-FILM HOT-PFACTOR
COLD-FOULING COLD-FILM COLD-PFACTOR

```
PROPERTIES    opsetname    keyword=value    [/ opsetname    keyword=value]
```

Optional keywords:

FREE-WATER SOLU-WATER HENRY-COMPS

```
FLASH-SPECS    sid    keyword=value
```

Optional keywords:

NPHASE PHASE FREE-WATER MAXIT TOL

Input Language Description for HTRIXIST

PARAM

Use to enter overall parameters for the block.

INPUT-FILE..... Name of the HTRI IST heat exchanger program input file

CREATE-FILE..... Determines whether to create the HTRI IST input file, if it does not currently exist:

	CREATE-FILE=NO	Does not create the HTRI IST input file.
	CREATE-FILE=YES	Creates the HTRI IST input file at the end of the simulation, if the file does not exist

HTRI-UNITS Determines which HTRI unit set will be used when creating a new input file:

HTRI-UNITS=US	Uses HTRI US engineering units
HTRI-UNITS=SI	Uses HTRI SI units
HTRI-UNITS=METRIC	Uses HTRI metric units

SAV-HOT-STRM Determines whether to save Aspen Plus hot-stream data in the HTRI IST input file:

SAV-HOT-STRM=NO	Does not write Aspen Plus hot-stream data to the HTRI IST input file (Default)
SAV-HOT-STRM=YES	Writes Aspen Plus hot-stream data to the HTRI IST input file, at the end of the simulation

SAV-CLD-STRM Determines whether to save Aspen Plus cold-stream data in the HTRI IST input file:

SAV-CLD-STRM=NO	Does not write Aspen Plus cold-stream data to the HTRI IST input file (Default)
SAV-CLD-STRM=YES	Writes Aspen Plus cold-stream data to the HTRI IST input file, at the end of the simulation

FEEDS, PRODUCTS, DECANT_STREAMS

Use to identify inlet and outlet streams. You must identify hot and cold inlets and outlets, and any water decant streams.

HOT-SIDE Stream ID for the hot side

COLD-SIDE Stream ID for the cold side

HOT-PCURVE, COLD-PCURVE

Use to set parameters to control the generation of property curves for the HTRI heat exchanger program IST.

GENERATE Determines which program generates property curves:

GENERATE=YES	Aspen Plus generates property curves using parameters supplied by the HTRI IST program. (Default)
GENERATE=-NO	Property curves are read from the HTRI IST input file.

UPDATE Controls how often Aspen Plus generates property curves:

UPDATE=ALWAYS	Calculates property curves at every block execution (Default)
UPDATE=NEVER	Calculates property curves only at the first block execution
UPDATE=AS-NEEDED	Calculates property curves if the range of the curve or the ends deviate by more than INDP-DEV from the previous execution

SAVE-CURVE Determines whether to save the Aspen Plus property curve in the HTRI IST input file:

SAVE-CURVE=NO	Does not write the property curve to the HTRI IST input file (Default)
SAVE-CURVE=YES	Writes the property curve to the HTRI IST input file, at the end of the simulation

INDP-DEV Controls the percent deviation Aspen Plus tolerates in the independent variable, before Aspen Plus recalculates the property curve

HTRI-INPUTS

Use to set HTRI input values. These values can be used in Aspen Plus simulation tools such as sensitivity, design-specs, and datafit.

HOT-FOULING..... Fouling factor for the hot-side stream

HOT-FILM ..... Film coefficient for the hot-side stream

HOT-PFACTOR..... Correction factor applied to the calculated hot-side pressure drop

COLD-FOULING..... Fouling factor for the cold-side stream

COLD-FILM..... Film coefficient for the cold-side stream

COLD-PFACTOR..... Correction factor applied to the calculated cold-side pressure drop

PROPERTIES Use to override global or flowsheet section property specifications. You can use different physical property option sets for the hot and cold sides of the exchanger. If you supply one set of property specifications, Aspen Plus uses the set for both hot-side and cold-side calculations. If you supply two sets, Aspen Plus uses the first set for the hot side, and the second set for the cold side. If you enter an option set name, you must also enter the name in the PROPERTIES paragraph.
(See Chapter 8.)

FLASH-SPECS Use to specify flash options for the hot or cold side of the heat exchanger. For each side of the heat exchanger, you can specify vapor phase, liquid phase, two-phase flash, or three-phase flash calculations.

sid..... Outlet stream ID. Flash specifications for the outlet stream apply to all flash calculations on that side of the heat exchanger.

NPHASE ..... Number of phases in MIXED substream:

NPHASE=1	One-phase calculation
NPHASE=2	Two-phase flash (Default)
NPHASE=3	Three-phase flash

PHASE..... Specifies the phase when NPHASE=1

PHASE=V	Vapor (Default)
PHASE=L	Liquid
PHASE=S	Solid. Use for electrolytes system only.

FREE-WATER..... Use to override the free-water option established by the SIM-OPTIONS paragraph. (See Chapter 45.) Or use to override the free-water option established by the BLOCK-OPTIONS sentence of the BLOCK paragraph. (See Chapter 11.)

FREE-WATER=NO	Does not perform free-water calculations
FREE-WATER=YES	Performs free-water calculations

MAXIT..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph. See Chapter 45.)

TOL..... Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph. See chapter 45.)

Accessing Variables in HTRIXIST

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables
HTRI-INPUTS	HOT-FOULING, HOT-FILM, HOT-PFACTOR, COLD-FOULING, COLD-FILM, COLD-PFACTOR

Block Results

Description	Sentence	Variable
Total heat load transferred between the process streams in the heat exchanger	UNIT-RESULT	HEAT-DUTY
Total outside surface area of all tubes in the heat exchanger	UNIT-RESULT	TOTAL-AREA
Total outside surface area of the tubes that is available for heat transfer	UNIT-RESULT	EFFECT-AREA
Overall rate at which heat is transferred from the hot fluid to the cold fluid	UNIT-RESULT	OVERALL-COEF
Effective temperature difference for the entire exchanger	UNIT-RESULT	EFF-DELTA-T
Correction factor applied to the log-mean temperature difference, to correct for flow arrangements that are not true counter-current	UNIT-RESULT	LMTD-CORRECT
Temperature of the tube wall on the outside of the tubes	SHELL-RESULT	WALL-TEMP
Average temperature of the fouling layer on the outer surface of the tubes	SHELL-RESULT	SKIN-TEMP
Pressure drop of the fluid flow on the shell side of the exchanger, without fouling	SHELL-RESULT	CLEAN-DP
Pressure drop of the fluid flow on the shell side of the exchanger, with fouling present	SHELL-RESULT	DIRTY-DP
Pressure drop of the shell-side fluid flow through the baffle windows	SHELL-RESULT	WINDOW-DP
Pressure drop of the shell-side fluid flow through the inlet and outlet zones of the exchanger	SHELL-RESULT	ENDS-DP
Pressure drop of the flow of the shell-side fluid across the bundle	SHELL-RESULT	CROSSFLOW-DP
Heat-transfer coefficient between the bulk fluid and the fluid film on the heat-transfer surface, for the shell side of the exchanger	SHELL-RESULT	BULK-COEF
Heat-transfer coefficient at the tube wall, for the shell side of the exchanger	SHELL-RESULT	WALL-COEF
Heat-transfer coefficient for the transfer of heat between the shell-side fluid passes, across the longitudinal baffle	SHELL-RESULT	LB-BULK-COEF
Overall thermal resistance to heat transfer on the outside of the tubes	SHELL-RESULT	THERM-RESIST
Thermal resistance to heat transfer of the fouling layer on the outside of the tubes	SHELL-RESULT	FOUL-RESIST
Thickness of the fouling layer on the outside of the tubes	SHELL-RESULT	FOUL-THICK
Correction factor applied to the shell-side heat-transfer coefficient, to reflect the presence of fins on the tubes	SHELL-RESULT	FIN-CORR

continued

Block Results (continued)

Description	Sentence	Variable
Correction factor applied to the log-mean temperature difference, to account for thermal leakage across the longitudinal baffle on the shell side of the exchanger	SHELL-RESULT	LBAF-CORR
Nominal velocity of that portion of the shell-side fluid that flows across the bundle	SHELL-RESULT	CROSSFLOW-VL
Nominal velocity of the shell-side fluid that flows through the baffle windows	SHELL-RESULT	WINDOW-VL
Velocity of the shell-side fluid that flows across the bundle, at a temperature midway between the inlet and outlet temperatures of the exchanger	SHELL-RESULT	MIDPOINT-VL
rho-v^2 (density x velocity^2) for the shell-side fluid, as it enters the shell	SHELL-RESULT	SHL-IN-RHV2
rho-v^2 (density x velocity^2) for the shell-side fluid, as it exits the shell	SHELL-RESULT	SHL-OUT-RHV2
rho-v^2 (density x velocity^2) for the shell-side fluid, as it enters the bundle	SHELL-RESULT	BND-IN-RHV2
rho-v^2 (density x velocity^2) for the shell-side fluid, as it exits the bundle	SHELL-RESULT	BND-OUT-RHV2
Heat-transfer efficiency of the additional surface area provided by the external fins on the tubes	SHELL-RESULT	FIN-EFF
Temperature of the tube wall on the inside of the tubes	TUBE-RESULT	WALL-TEMP
Temperature of the fouling layer on the inside of the tubes	TUBE-RESULT	SKIN-TEMP
Pressure drop of the fluid on the inside of the tubes, assuming no fouling is present	TUBE-RESULT	CLEAN-DP
Pressure drop of the fluid on the inside of the tubes, assuming fouling is present	TUBE-RESULT	DIRTY-DP
Heat-transfer coefficient between the bulk fluid and the fluid film, for the tube side of the exchanger	TUBE-RESULT	BULK-COEF
Heat-transfer coefficient at the tube wall on the tube side of the exchanger	TUBE-RESULT	WALL-COEF
Thermal resistance to heat transfer for the tube-side fluid	TUBE-RESULT	THERM-RESIST
Thermal resistance to heat transfer due to fouling on the tube side of the exchanger	TUBE-RESULT	FOUL-RESIST
Thickness of fouling layer on the tube side of the exchanger	TUBE-RESULT	FOUL-THICK
Velocity of the tube-side fluid as it enters the tubes, immediately after entering the bundle	TUBE-RESULT	INLET-VL
Velocity of the tube-side fluid as it exits the tubes, prior to leaving the bundle	TUBE-RESULT	OUTLET-VL
Velocity of the tube-side fluid, at a temperature midway between the inlet and outlet temperatures of the exchanger	TUBE-RESULT	MIDPOINT-VL

14 Shortcut Distillation

This chapter describes the input language for the shortcut distillation models. The models are:

Model	Description	Purpose	Use
DSTWU	Shortcut distillation design	Determine minimum reflux ratio, minimum number of stages, and either actual reflux ratio or actual number of stages using Winn-Underwood-Gilliland method	Columns with one feed and two product streams
DISTL	Shortcut distillation rating	Determine separation based on reflux ratio, number of stages, and distillate-to-feed ratio using Edmister method	Columns with one feed and two product streams
SCFRAC	Shortcut distillation for complex petroleum fractionation units	Determine product composition and flow, number of stages per section, and heat duty using fractionation indices	Complex columns, such as crude units and vacuum towers

DSTWU: Shortcut Distillation Design

Input Language for DSTWU

```
BLOCK    blockid    DSTWU
PARAM    keyword=value
```

Keywords:

LIGHTKEY RECOVL HEAVYKEY RECOVH PTOP PBOT NSTAGE RR

Optional keywords:

RDV PACK-HEIGHT MAXIT FLASH-MAXIT FLASH-TOL TEMP-TOL K-TOL PLOT

```
PLOT    keyword=value
```

Optional keywords:

LOWER UPPER INCR NPOINT HIGH-PRECISION LINES WIDE

Input Language Description for DSTWU

PARAM

Use to specify the column operating conditions, configuration, and optional convergence parameters. You must specify the recovery of the light and heavy keys, reboiler and condenser pressures, and either reflux ratio or number of theoretical stages. You can also specify whether a plot of reflux ratio versus number of stages is to be produced. Enter plot parameters in the PLOT sentence.

LIGHTKEY		Light key component ID
RECOVL		Recovery of light key component in distillate (moles light key in distillate/moles light key in feed)
HEAVYKEY		Heavy key component ID
RECOVH		Recovery of heavy key component in distillate (moles heavy key in distillate/moles heavy key in feed)
PTOP		Condenser pressure
PBOT		Reboiler pressure
NSTAGE		Number of theoretical stages, including condenser and reboiler
RR	**RR > 0**	Desired reflux ratio
	RR < -1	Desired reflux ratio is $\left\|\mathrm{RR}\right\|$ times the minimum reflux ratio.
RDV		Molar vapor fraction of distillate (Default=0)
PACK-HEIGHT		Column packing height, used to compute HETP (Height Equivalent of a Theoretical Plate)
MAXIT		Maximum number of iterations in minimum stages calculation (Default=50)
FLASH-MAXIT		Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

FLASH-TOL	Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	
TEMP-TOL	Tolerance on distillate and bottoms temperature in minimum stages calculation (Default=0.2K)	
K-TOL	Tolerance on light and heavy key component K-values in minimum stages calculation (Default=0.05)	
PLOT	**PLOT=YES**	Produces print-plots and tables of actual reflux ratio versus actual number of stages.
	PLOT = NO	Does not produce print-plots and tables. (Default)
	You specify print-plot specifications in the PLOT sentence.	

PLOT

Use to specify the print-plot of actual reflux ratio versus actual number of stages. Use either NPOINT or INCR.

LOWER	Initial stage number for the plot and the tables (Default=actual number of stages – 5)	
UPPER	Final stage number for the plot and the tables (Default=actual number of stages + 5)	
INCR	Increment size for number of stages	
NPOINT	Number of point values (Default=11)	
HIGH-PRECISION	**HIGH-PRECISION=YES**	Prints seven significant digits in tables
	HIGH-PRECISION=NO	Prints five significant digits in tables (Default)
LINES	Number of rows of values to print in tables before printing a grid line. If LINES=0, no grid lines are printed. Must be between 0 and 35. (Default=5)	
WIDE	Plot width option.	
	WIDE=YES	Produces wide (132 column) plots.
	WIDE=NO	Produces standard (80 column) plots. (Default)

Accessing Variables in DSTWU

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables
PARAM	RECOVL, RECOVH, PTOP, PBOT, RDV, NSTAGE, RR, MAXIT, PACK-HEIGHT, FLASH-MAXIT, FLASH-TOL, TEMP-TOL, K-TOL

Block Results

Description	Sentence	Variable
Minimum reflux ratio	RESULTS	MIN-REFLUX
Actual reflux ratio	RESULTS	ACT-REFLUX
Minimum number of stages	RESULTS	MIN-STAGES
Actual number of stages	RESULTS	ACT-STAGES
Actual number of stages in rectifying section	RESULTS	RECT-STAGES
Height equivalent of a theoretical plate	RESULTS	HETP
Reboiler duty	RESULTS	REB-DUTY
Condenser duty	RESULTS	COND-DUTY

DISTL: Shortcut Distillation Rating

Input Language for DISTL

```
BLOCK    blockid    DISTL
PARAM    keyword=value
```

Keywords:

NSTAGE FEED-LOC RR PTOP PBOT D:F

Optional keywords:

COND-TYPE MAXIT FLASH-MAXIT FLASH-TOL TEMP-TOL

Input Language Description for DISTL

PARAM

Use to specify column operating conditions, configuration, and optional convergence parameters. You must specify the number of theoretical stages, feed stage number, reflux ratio, condenser type, distillate-to-feed ratio, condenser pressure, and reboiler pressure.

NSTAGE..... Number of theoretical stages, including condenser and reboiler

FEED-LOC..... Feed stage location (numbered from the top including the condenser)

RR..... Molar reflux ratio

PTOP	Condenser pressure	
PBOT	Reboiler pressure	
D:F	Moles in distillate/moles in feed	
COND-TYPE	**COND-TYPE=TOTAL**	Total condenser (Default)
	COND-TYPE=PARTIAL	Partial condenser
MAXIT	Maximum number of iterations (Default=60)	
FLASH-MAXIT	Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	
FLASH-TOL	Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	
TEMP-TOL	Tolerance on distillate and bottoms temperature (Default=0.005 K)	

Accessing Variables in DISTL

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables
PARAM	NSTAGE, FEED-LOC, RR, PTOP, PBOT, D:F, MAXIT, FLASH-MAXIT, FLASH-TOL, TEMP-TOL

Block Results

Description	Sentence	Variable
Reboiler duty	RESULTS	REB-DUTY
Condenser duty	RESULTS	COND-DUTY

SCFRAC: Shortcut Distillation for Complex Columns

Input Language for SCFRAC

```
BLOCK    blockid    SCFRAC
PARAM    keyword=value
```

Optional keywords:

MAXIT TOL FLASH-MAXIT FLASH-TOL MAX-FINDEX

```
CONDENSER    keyword=value
```

Optional keywords:

PRES RDV TEMP DEGSUB

PRODUCTS	**sid**	**secno**	*keyword=value*

Keywords:

TYPE PRES

Optional keywords:

basis-FLOW-EST basis-FEED-FRAC

STEAM	**sid**	*keyword=value*

Keywords:

STEAM:PROD TEMP PRES

SPEC	**specno**	**spectype**	**value**	*keyword=value*

Spectypes:

basis-FRAC basis-RECOV basis-FLOW PROP PROP-DIFF PROP-RATIO

Keywords:

STREAM BASE-STREAM COMPS PROPERTY BASE-PROPERTY FLASH

FINDEX secno findex / . . .
FI-HEAVY secno fi-heavy / . . .
FI-RATIO secno fi-ratio / . . .
FINDEX-EST secno findex-est / . . .

Input Language Description for SCFRAC

PARAM

Use to enter values for convergence parameters.

MAXIT..... Maximum number of iterations (Default=50)

TOL..... Relative tolerance on the root-mean-square residuals of the product specifications (Default=$1x10^{-4}$)

FLASH-MAXIT..... Maximum number of iterations for flash calculations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

FLASH-TOL..... Flash tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

MAX-FINDEX..... Maximum value allowed for fractionation index (Default=10)

CONDENSER

Use to enter condenser specifications. You can specify pressure and either RDV (molar vapor distillate flow/total distillate flow) or temperature. For total condensers (RDV=0), you can specify the number of degrees the product is subcooled. If you do not use the CONDENSER sentence, SCFRAC assumes the distillate is vapor and pressure is the top section pressure.

PRES..... Condenser pressure (Default=top section pressure)

RDV..... Distillate vapor fraction (Default=1)

TEMP..... Temperature of product stream. You cannot use both TEMP and RDV.

DEGSUB..... Number of degrees product is subcooled. You can specify DEGSUB if RDV=0. (Default=0)

PRODUCTS

Use to enter pressure, temperature, and flow estimates for product streams. You must enter flow rate estimates for all products unless you specify the flow. You can give flow estimates directly or as a fraction of the feed. For products from the top section, you must enter TYPE to indicate whether the stream is the overhead (distillate) or the bottoms stream from that section.

sid..... Stream ID

secno ..... Section number

TYPE ..... Product type for top section:

TYPE=O	Overhead
TYPE=B	Bottoms (Default)

PRES ..... Pressure

basis-FLOW-EST..... Estimate of stream flow rate on a MOLE, MASS, or STDVOL basis

basis-FEED-FRAC ..... Estimate of stream flow as a fraction of feed on a MOLE, MASS, or STDVOL basis

STEAM

Use to enter the steam to product flow ratio for all products except the distillate product. Also use to enter steam temperature and pressure. The sum of all stripping steam flows is stored in the optional second inlet stream for the block to maintain a mass balance.

sid..... Product stream ID

STEAM:PROD..... Steam to product ratio in mass/bbl (Default=2.27 kg/bbl) (Units keyword is MASS)

TEMP..... Steam temperature

PRES ..... Steam pressure

SPEC

Use to provide the 2*(n – 1) specifications for the column. Do not impose more than two specifications on a given product stream. If the number of specifications for a section is insufficient, use the FINDEX sentence to specify the fractionation index for the section.

specno ..... Specification number

spectype ..... Specification type. The following types are available:

basis-FRAC	Purity of a product stream (specified by STREAM). FRAC=Σx_i Where: x = Component fraction, on a MOLE, MASS, or STDVOL basis i = Component in the COMPS list
basis-RECOV	Component recovery. RECOV=$\Sigma f_{ij}/\Sigma f_{ik}$ Where: f = Component flow rate, on a MOLE, MASS, or STDVOL basis i = Component in the COMPS list j = Product stream specified by STREAM k = Feed stream
basis-FLOW	Flow rate on a MOLE, MASS, or STDVOL basis of a group of components (specified by COMPS), in a product stream (specified by STREAM). The default for COMPS is all components.
PROP	Property value (specified by PROPERTY) for a product stream (specified by STREAM)

	PROP-DIFF	PROPERTY minus BASE-PROPERTY. PROPERTY is the property of a product stream (specified by STREAM). BASE-PROPERTY is the property of a product stream (specified by BASE-STREAM).
	PROP-RATIO	PROPERTY divided by BASE-PROPERTY. PROPERTY and BASE-PROPERTY are as defined for PROP-DIFF.

value ..... Value of specification

STREAM ..... Product stream ID

BASE-STREAM ..... Product stream ID

COMPS ..... List of component IDs

PROPERTY ..... ID of a property set defined by a PROP-SET paragraph consisting of a single scalar property. (See Chapter 41.)

BASE-PROPERTY ..... ID of a property set defined by a PROP-SET paragraph consisting of a single scalar property. (See Chapter 41.)

FLASH	**FLASH=YES**	Performs flash calculations at each iteration to determine stream temperature. This option is needed only if property for *spectype* PROP, PROP-DIFF, or PROP-RATIO is temperature-dependent.
	FLASH=NO	Does not perform flash calculations at each iteration (Default)

FINDEX

Use to enter the fractionation index for each column section. Normally, the value applies to all components. If you enter FI-HEAVY, then the FINDEX value applies only to the light components for the section.

secno ..... Section number

findex ..... Fractionation index (Default=2)

FI-HEAVY

Use to enter the fractionation index for heavy components for the section. Do not enter FI-HEAVY if you specified FI-RATIO.

secno ..... Section number

fi-heavy ..... Fraction index for heavy components for the section

FI-RATIO

Use to enter the ratio of the fractionization index for heavy components for the section to that for light components. Do not enter FI-RATIO if you specified FI-HEAVY.

secno ..... Section number

fi-ratio ..... Ratio of the fractionization index for heavy components for the section to that for light components

FINDEX-EST

Use to enter an estimate for fractionization index. Applies to light components if you specified FI-HEAVY or FI-RATIO. As a first approximation, the fractionation index can be estimated as one-half of the number of theoretical stages, or from the correlation developed by Jakob (1971) for middle-eastern crude.

secno ..... Section number

findex-est ..... Estimate of the fractionization index (Default=2)

Accessing Variables in SCFRAC

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1
PARAM	MAXIT, TOL, FLASH-MAXIT, FLASH-TOL, MAX-FINDEX	—
CONDENSER	PRES, RDV, TEMP, DEGSUB	—
PRODUCTS	PRES, basis-FLOW-EST, basis-FEED-FRAC	sid
STEAM	STEAM:PROD, TEMP, PRES	sid
SPEC	VALUE	specno
FINDEX	FINDEX	secno
FINDEX-EST	FIEST	secno
FI-HEAVY	FIHEAVY	secno
FI-RATIO	FIRATIO	secno

Block Results

Description	Sentence	Variable†	ID1
Fractionation index	PROFILE	FINDEX	secno
Number of theoretical stages	PROFILE	STAGE	secno
Duty	PROFILE	DUTY	secno
Steam flow rate	PROFILE	STEAM-FLOW	secno

† You can also access variables using the VECTOR-DEF sentence. See Chapter 29.

15 Rigorous Distillation

This chapter describes the input language for the rigorous distillation models. The models are:

Model	Description	Purpose	Use to model
RADFRAC	Rigorous fractionation	Rigorous rating and design calculations for single columns	Ordinary distillation, absorbers, strippers, extractive and azeotropic distillation, three-phase distillation, and reactive distillation
MULTIFRAC	Rigorous fractionation for complex columns	Rigorous rating and design calculations for multiple columns of any complexity	Heat integrated columns, air separation columns, absorber/stripper combinations, ethylene plant primary fractionator/quench tower combinations, and petroleum refining applications
PETROFRAC	Petroleum refining fractionation	Rigorous rating and design calculations for complex columns in petroleum refining applications	Preflash tower, atmospheric crude unit, vacuum unit, catalytic cracker main fractionator, delayed coker main fractionator, vacuum lube fractionator, and ethylene plant primary fractionator/ quench tower combinations

See also Chapter 16 for input language used with these models for rating and sizing calculations for trays and packing, and Chapter 17 for input language used with RADFRAC for the RateSep rate-based distillation feature.

RADFRAC: Rigorous Fractionation

Input Language for RADFRAC

```
BLOCK blockid RADFRAC
SUBOBJECTS PUMPAROUND=paid
PROP-SECTIONS stage1 stage2 opsetname keyword=value
```

Keywords:

FREE-WATER SOLU-WATER HENRY-COMPS CHEMISTRY PHASE-EQM

```
PARAM keyword=value
```

Keywords:

NSTAGE NPA NPHASE

Optional keywords:

ALGORITHM EFF INIT-OPTION SOLID-BAL HYDRAULIC P-UPDATE P-FIX DAMPING MAXOL TOLOL ABSORBER CMAXNI0 CMAXNI1 DSMETH DTMAX EFF-FLASH FLASH-MAXIT FLASH-TOL FLASH-VFRAC FMINFAC GAMMA-MODEL HMODEL1 HMODEL2 ILMETH JMETH KBBMAX KMODEL L2-CUTOFF L2-GAMMA LL-MAXIT LL-METH MAX-BROY MAX-SIZE MAXIL MAXIP PROD-FLASH QMAXBWIL QMAXBWOL QMINBWIL QMINBWOL RMSOL0 RMSOL1 RMSOLJ STOR-FACTOR TOLILFAC TOLILMIN TOLIL0 FLASH-TOLIL PHEQM-FORM RADIUS-FRAC

```
COL-CONFIG keyword=value
```

Keywords:

CONDENSER REBOILER KEY-SELECT

```
FEEDS sid stage [feed-conv] / ...
PRODUCTS sid stage [phase] [basis-FLOW=value] / ...
SDRAW:FEED sid ratio keyword=value / ...
```

Keywords:

STREAMS COMPS

```
PSEUDO-STREAM sid stage keyword=value / ...
```

Keywords:

PHASE MOLE-FLOW PA STATE

```
P-SPEC stage pres / ...
```

COL-SPECS *keyword=value*

Keywords:

basis-RDV T1 basis-D basis-B D:F B:F basis-D:F basis-B:F basis-L1 basis-VN basis-RR basis-BR Q1 QN

Optional keywords:

RW DP-STAGE DP-COL DP-COND HTLOSS

PDROP-SEC secno stage1 stage2 pdrop / . . .
DB:F-PARAMS *keyword=value*

Keywords:

STREAMS COMPS

SC-REFLUX *keyword=value*

Keywords:

DEGSUB TEMP

Optional keyword:

OPTION

THERMOSYPHON *keyword=value*

Keywords:

PRES TEMP DELT VFRAC basis-FLOW RETURN-CONV

PUMPAROUND paid stage1 stage2 *keyword=value*

Keywords:

DRAW-PHASE TYPE basis-FLOW TEMP DELT DUTY VFRAC PRES NPHASE RETURN-PHASE FEED-CONV QSTREAM-IN QSTREAM-OUT

HEATERS stage duty / . . .
COOLANT stage cid opsetname *keyword=value*

Keywords:

basis-FLOW UA TEMP PRES PHASE basis-CP

HTLOSS-SEC secno stage1 stage2 HTLOSS-SEC=value HTLOSS-VAP=value / . . .
HTLOSS HTLOSS-LIQ=value HTLOSS-VAP=value
COMP-EFF stage cid eff / . . .
STAGE-EFF stage eff / . . .
STEFF-SEC secno stage1 stage2 eff / . . .
DECANTERS stage *keyword=value*

Keywords:

L1-SPEC L2-SPEC

Optional keywords:

TEMP DEGSUB DECANT-SOLID

L2-COMPS cid-list
L2-STAGES stage1 stage2 / . . .
L1-RETURN stage1 stage2 l1-rfrac / . . .

```
L2-RETURN   stage1   stage2   l2-rfrac  / ...
L1-COMP-EFF   stage   cid   eff  / ...
L2-COMP-EFF   stage   cid   eff  / ...
L1-STAGE-EFF   stage   eff  / ...
L2-STAGE-EFF   stage   eff  / ...
KLL-STAGES   kllno   stage1   stage2  / ...
basis-KLL   KLL-NO=value   KLL-CID=cid   KLL-A=value   [KLL-B=value]   &
      [KLL-C=value]   [KLL-D=value]
REAC-STAGES   stage1   stage2   reacid  / ...
HOLD-UP   stage1   stage2   keyword=value  / ...
```

Keywords:

basis-LHLDP basis-VHLDP

```
RES-TIME   stage1   stage2   keyword=value  / ...
```

Keywords:

LTIME VTIME

```
CONVERSION   stage   reacno   frac
T-EST   stage   temp  / ...
X-EST   stage   cid   x  / ...
Y-EST   stage   cid   y  / ...
L-EST   stage   mole-flow  / ...
V-EST   stage   mole-flow  / ...
VL-EST   stage   mole-ratio  / ...
REPORT   reportopt-list
```

Special report options:

NOPROFILE NOCOMPS NOHYDRAULIC NOENTH NOSPLITS STDVPROF TARGET HYDANAL EXTHYD INT-PROF INT-AREA BULKRXN DIFF-COE MT-RATE MT-COEFF HT-RATE HT-COEFF FILMRXN S-DIMLES V-DIMLES

```
SPC-OPTIONS   keyword=value
```

Optional keywords:

EFF D B RR L1 BR VN Q1 QN L V Q-STAGE WL WV SPEC SC-REFLUX

```
SPC-OPTION2   keyword=value
```

Optional keywords:

PRES FEEDDP FEEDOPEN CS-ALLBASIS SPLIT-ALL

```
KEY-COMP   secno   stage1   stage2   LIGHT-KEY=cid-list   HEAVY-KEY=cid-list
KEY-TOL   keyword=value
```

Optional keywords:

KVAL-TOL COMP-TOL SPF-LIMIT STG-SPAN EXCLD-KEY EXG-TREF

```
CONVERGENCE   keyword=value
```

Optional keywords:

MAN-3P-PASS STABLE-ITER STABLE-METH PROP-DERIV NQ-PROF-MAX NQ-FOPT-METH NQ-TOLOL NQ-TOLOBJ

TRAY-REPORT *keyword=value*

Optional keywords:

TRAY-OPTION FORMAT ORDER PROPERTIES WIDE

TRAY-REPOPT *keyword=value*

Optional keywords:

FLOW-OPTION

INCL-TRAYS [stage1] [stage2] / ...
COND-HCURVE curveno *keyword=value*
REB-HCURVE curveno *keyword=value*
PA-HCURVE paid curveno *keyword=value*

Optional keywords:

INDEP-VAR LIST NPOINT INCR HEADING PROPERTIES PRES-PROFILE PDROP PRINT-PLOT HIGH-PRECISION LINES X-SCALE Y-SCALE
WIDE GRID INTERPOLATE

VARY varyno vartype lb ub [step] *keyword=value*

Vartypes:

basis-RDV basis-D basis-B D:F B:F basis-D:F basis-B:F basis-L1 basis-VN basis-RR basis-BR Q1 QN RW basis-LPROD basis-VPROD
DUTY FEED-FLOW HEAT-STREAM MURPHREE TREB DTREB VREB basis-RFLOW L1-SPEC L2-SPEC basis-PA-FLOW PA-TEMP PA-DELT PA-DUTY PA-VFRAC SDRAW:FEED

Keywords:

STAGE STREAM STAGE1 STAGE2 COMPS PA

SPEC specno spectype value [scale] [weight] *keyword=value*

Spectypes:

basis-FRAC basis-RECOV basis-FLOW basis-RATIO TEMP PROP PROP-DIFF PROP-RATIO basis-D basis-B basis-L1 basis-VN basis-RR basis-BR Q1 QN

Keywords:

STAGE BASE-STAGE COMPS BASE-COMPS STREAMS BASE-STREAMS PROPERTY BASE-PROPERTY DEC-STREAM

Optional keywords:

PHASE BASE-PHASE

DIAGNOSTICS *keyword=value*

Keywords:

MAIN OLVAR1 OLVAR2 CMBAL EMBAL DESIGN TERM TXYEST

NQ-CURVE *keyword=value*

Keywords:

CURVE-NO NSTAGE-MIN NSTAGE-MAX FEED OBJECT-FUNC QR-QC-COST

Optional keywords:

NSTAGE-STEP RR-MIN LMT-FROM-TOP LMT-FROM-BOT

NQCUR-FOPT *keyword=value*

Keywords:

CURVE-NO SID REMAIN-OPT

NQCUR-SOPT *keyword=value*

Keywords:

CURVE-NO SID SDRAW-OPT

NQCUR-PAOPT *keyword=value*

Keywords:

CURVE-NO IC-STREAM PA-OPT

NQCUR-DECTOP *keyword=value*

Keywords:

CURVE-NO STAGE DECT-OPT

PLOT plotno plot-list comp-plot=groupid-list *keyword=value*

Plot-list options:

TEMP PRES LRATE VRATE VL-RATIO LL-RATIO

Comp-plot options:

X X1 X2 Y KVL KVL1 KVL2 KLL REL-VOL S-PLOT

Optional keywords:

BASE-COMP S-OPTION HEAVY-KEY BASIS ORDER PLOT-HEADING WIDE

SUBROUTINE KLL=subrname
KLL-USER stage1 stage2 / . . .
KLL-VECS *keyword=value*

Keywords:

NINT NREAL

KLL-INT VALUE-LIST=values
KLL-REAL VALUE-LIST=values
USERK-VECS *keyword=value*

Keywords:

NINT NREAL NIWORK NWORK

USERK-INT VALUE-LIST=values
USERK-REAL VALUE-LIST=values
STG-UTL *stage utilityid*
PA-UTL *pid utilityid*
UTILITIES *keyword=value*

Optional keywords:

COND-UTIL REB-UTIL

PARAM2 *keyword=value*

Keywords:

SALTS SAT-LIMIT

Input Language Description for RADFRAC

SUBOBJECTS

Use to enter a list of IDs for pumparounds. The IDs are character strings of up to eight characters long. They are used for referencing pumparounds in other input statements. If you do not enter IDs using the SUBOBJECTS statement, pumparounds are referenced by sequential integer numbers.

PUMPAROUND..... List of pumparound IDs

PROP-SECTIONS

Use to specify property options for a column segment, the thermosyphon reboiler, or a decanter. PROP-SECTIONS overrides the PROPERTIES sentence for a column segment, the thermosyphon reboiler, or a decanter. The input language for PROP-SECTIONS is the same as for the PROPERTIES sentence, except that PROP-SECTIONS requires that you specify the column segment. See Chapter 11, for more information about the PROPERTIES sentence. Column initialization calculations are always performed using the specifications in the PROPERTIES sentence, regardless of the specifications given in the PROP-SECTIONS sentence. Therefore, it is important that the property option in the PROPERTIES sentence gives reasonable property representation at the average condition of the column. Any option set name entered in the PROP-SECTIONS sentence must also be named in the PROPERTIES sentence. (For more information about specifying an option set, see Chapter 8.)

stage1..... For column segment, *stage1*=starting stage number of column segment; for decanter, *stage1*=decanter stage number; for thermosyphon reboiler, *stage1*=bottom stage number.

stage2..... For column segment, *stage2*=ending stage number of column segment; for decanter, enter D in this position; for thermosyphon reboiler, enter R.

opsetname..... Property option set used for column segment

PHASE-EQM ..... Phase equilibrium for which property option set specification is to be used:

PHASE-EQM=VLL	Vapor-liquid1-liquid2 equilibrium (Default)
PHASE-EQM=VL1	Vapor-liquid1 equilibrium
PHASE-EQM=LL	Liquid1-liquid2 equilibrium

PARAM

Use to enter configuration and operating specifications for the column. You must enter the number of stages and pumparounds. You can also specify algorithm option, efficiency type, and optional parameters.

NSTAGE..... Number of stages, including condenser and reboiler. Must be greater than 1. The convention used in RADFRAC is to number the stages from the top down, starting with the condenser.

NPA..... Number of pumparounds

NPHASE ..... Number of phases to be considered in distillation calculations. Specify 2 for vapor-liquid and 3 for vapor-liquid1-liquid2 calculations. If you specify FREE-WATER=YES and NPHASE=2, free-water calculation is performed for the condenser.

ALGORITHM ..... Algorithm convergence options:

ALGORITHM=STANDARD	Normal algorithm. Recommended for most applications. (Default)
ALGORITHM=SUM-RATES	Recommended for petroleum and petrochemical applications involving wide-boiling mixtures. Allowed for NPHASE=2 only.
ALGORITHM=NONIDEAL	Recommended for highly nonideal columns. You cannot specify ALGORITHM=NONIDEAL and FREE-WATER=YES when NPHASE=2.
ALGORITHM=NEWTON	Recommended for azeotropic distillation columns

EFF..... Type of efficiency specified using keywords: COMP-EFF, STAGE-EFF, L1-COMP-EFF, L2-COMP-EFF, L1-STAGE-EFF, or L2-STAGE-EFF

EFF=VAPOR	Vaporization efficiency (Default)
EFF=MURPHREE	Murphree efficiency
EFF=TH-MURPHREE	Thermal-Murphree efficiency

INIT-OPTION ..... Initialization options:

INIT-OPTION=STANDARD	Standard initialization (Default)
INIT-OPTION=CRUDE	Special initialization designed for wide-boiling and multidraw columns
INIT-OPTION=CHEMICAL	Special initialization designed for narrow-boiling chemical systems
INIT-OPTION=AZEOTROPIC	Special initialization designed for azeotropic distillation columns, such as ethanol dehydration using benzene as the entrainer
INIT-OPTION=CRYOGENIC	Special initialization designed for cryogenic applications, such as air separation

SOLID-BAL..... Solids handling options:

SOLID-BAL=STAGE	Handles solids rigorously in stage-by-stage mass and energy balance. All flow specifications must include solids.
SOLID-BAL=OVERALL	Removes solids from feeds and combines them with liquid bottoms to satisfy overall block mass and energy balance. Flow specifications must not include solids. (Default)

HYDRAULIC..... Flag to specify whether to perform calculations of hydraulic parameters (for example, flow parameter, reduced vapor throughput, tray loadings, and various transport properties): YES or NO. (Default=NO)

P-UPDATE ..... Update pressure profile during column sizing and rating calculations: YES or NO. (Default=NO)

P-FIX ..... Pressure update option: TOP or BOTTOM. Keeps pressure at column top/bottom constant during pressure updating for column sizing and rating calculations. (Default=TOP)

DAMPING..... Damping factor used to stabilize convergence when excessive oscillation is observed in the convergence behavior:

DAMPING=NONE	No damping (Default)
DAMPING=MILD	Mild level of damping
DAMPING=MEDIUM	Medium level of damping

	DAMPING=SEVERE	Severe level of damping. You may need to increase the maximum number of outside loop iterations (keyword MAXOL) to achieve convergence.
MAXOL	Maximum number of outside loop iterations (Default=25)	
TOLOL	Outside loop convergence tolerance (Default=$1x10^{-4}$)	
ABSORBER	**ABSORBER=YES**	Recommended for absorber/stripper columns when you specify ALGORITHM=STANDARD. You must specify basis-RDV=1, Q1 and QN in the COL-SPECS statement.
	ABSORBER=NO	Use for all other cases (Default)
CMAXNI0	Maximum value of local gamma model parameters at infinite dilution. Use when ALGORITHM=NONIDEAL and GAMMA-MODEL=MARGULES. (Default=1.5)	
CMAXNI1	Maximum value of local gamma model parameters at mole fraction = 0.5. Use when ALGORITHM=NONIDEAL and GAMMA-MODEL=MARGULES. (Default=1.3)	
DSMETH	Design specification convergence method, allowed when ALGORITHM=NEWTON or ILMETH=NEWTON:	
	DSMETH=SIMULT	Simultaneous method (Default when ALGORITHM=NEWTON)
	DSMETH=NESTED	Nested-iteration method (Default when ILMETH=NEWTON)
DTMAX	Maximum allowed change in temperature per inside loop. Use when ABSORBER=YES or ILMETH=NEWTON. Default is selected based on column specifications.	
EFF-FLASH	Flashes product streams when efficiency is specified: YES or NO. (Default=NO)	
FLASH-MAXIT	Maximum number of feed flash iterations (Default=50)	
FLASH-TOL	Feed flash tolerance (Default=$1x10^{-4}$)	
FLASH-VFRAC	Vapor fraction of composite feed flash in reactive distillation initialization calculations. Default is calculated based on column specifications.	
FMINFAC	Minimum allowed value for stage flow as a fraction of the total feed. (Default=$1x10^{-5}$)	
GAMMA-MODEL	Local gamma model options. Use when ALGORITHM=NONIDEAL:	
	GAMMA-MODEL= COMBINED	Uses constant activity coefficient
	GAMMA-MODEL= MARGULES	Uses Margules activity coefficient model (Default)
HMODEL1	Basis for local enthalpy departure model:	
	HMODEL1=MOLE	Molar basis
	HMODEL1=MASS	Mass basis
	HMODEL1=PSEUDO-MASS	Pseudo-mass basis, using internally generated molecular weight
	(Default is selected based on column specifications)	
HMODEL2	Temperature dependence option for local enthalpy departure model:	
	HMODEL2=NO-TEMP	No temperature dependence

	HMODEL2=TEMP	Temperature dependence term is computed initially, and is then kept constant
	HMODEL2=UPDATE	Temperature dependence term is updated every iteration

(Default is selected based on column specifications)

ILMETH ..... Inside loop convergence methods. Do not use when ALGORITHM=NEWTON:

ILMETH=BROYDEN	Broyden quasi-Newton method. (Default for all algorithms except SUM-RATES)
ILMETH=WEGSTEIN	Bounded Wegstein method. (Not allowed when ALGORITHM=SUM-RATES)
ILMETH=NEWTON	Newton method. (Not allowed when ALGORITHM=SUM-RATES)
ILMETH=SCHUBERT	Schubert quasi-Newton method, with Powell's dogleg stabilization. Allowed when ALGORITHM=SUM-RATES only. (Default when ALGORITHM=SUM-RATES)

JMETH ..... Jacobian calculation method used only when ALGORITHM=SUM-RATES:

JMETH=INIT	Jacobian matrix is computed initially by numerical perturbation, then updated by the Broyden method (Default)
JMETH=RMSOL	Jacobian matrix is computed by numerical perturbation until outside loop RMS error is below RMSOLJ. Then the matrix is updated by the Broyden method.

KBBMAX ..... Maximum allowable slope value for local average K-value model (Default =-500)

KMODEL ..... Weighting option for local average K-value model:

KMODEL=Y	Vapor mole fraction
KMODEL=X	Liquid mole fraction
KMODEL=K	Vapor fraction/(1+K-value)

(Default is selected based on column specifications)

L2-CUTOFF ..... Mole fraction threshold for second phase key component (L2-COMPS). When only one-liquid phase is present, the phase is identified as the second-liquid phase if its mole fraction of L2-COMPS is greater than L2-CUTOFF. Use when NPHASE=3. (Default=0.5)

L2-GAMMA ..... Local activity coefficient model option for the second-liquid phase, when NPHASE=3 and ALGORITHM=NONIDEAL:

L2-GAMMA=CONSTANT	Uses constant activity coefficient
L2-GAMMA=MARGULES	Uses Margules activity coefficient model (Default)

LL-MAXIT ..... Maximum number of liquid-liquid phase-split calculations in the inside loop used when NPHASE=3. You can set LL-MAXIT to zero to suppress calculations in the inside loop. (Default=20)

LL-METH ..... Liquid-liquid phase splitting method:

LL-METH=GIBBS	Gibbs free energy minimization method (Default)
LL-METH=EQ-SOLVE	Equation solving method
LL-METH=HYBRID	Combination of Gibbs free energy minimization and equality of fugacities

MAX-BROY ..... Maximum number of variables converged by the Broyden method in the outside loop. You should not increase MAX-BROY beyond 500. (Default=200)

MAX-SIZE..... Maximum size for work space (in real words.) Use when ALGORITHM=NEWTON or ILMETH=NEWTON. (Default=$2x10^9$)

MAXIL..... Maximum number of inside loop iterations per outside loop (Default=10)

MAXIP..... Maximum number of initialization calculation passes. Use for ABSORBER=YES and three-phase calculations. Default is selected based on column specifications.

PROD-FLASH..... Flash type for product stream in PROP-SET and recycle stream convergence calculations:

PROD-FLASH=PV	Flash with stream pressure and vapor fraction as specifications
PROD-FLASH=TP	Flash with stream temperature and pressure as specifications

(Default is selected based on column specifications)

QMAXBWIL ..... Maximum value of bounded Wegstein acceleration parameter for inside loop convergence (Default=0.5)

QMAXBWOL ..... Maximum value of bounded Wegstein acceleration parameter for outside loop convergence (Default=0.5)

QMINBWIL..... Minimum value of bounded Wegstein acceleration parameter for inside loop convergence (Default=0)

QMINBWOL..... Minimum value of bounded Wegstein acceleration parameter for outside loop convergence (Default=0)

RMSOL0 ..... Threshold value of outside loop RMS error that must be achieved before design specification iterations are performed (Default=0.1)

RMSOL1 ..... Threshold value of outside loop RMS error below which Broyden method is used for selected variables (Default=0.1)

RMSOLJ..... Value of the outside loop error below which the inside loop Jacobian matrix is updated by the Broyden method. Use when ALGORITHM=SUM-RATES and JMETH=RMSOL.

STOR-FACTOR..... Storage multiplier to override the internally calculated workspace requirement when ALGORITHM=NEWTON or ILMETH=NEWTON (Default=1.5)

TOLILFAC..... Ratio of inside loop tolerance to outside loop RMS error. Default is calculated based on column specifications.

TOLILMIN ..... Minimum value of inside loop tolerance. Default is calculated based on column specifications.

TOLIL0..... Initial value of inside loop tolerance (Default=0.01)

FLASH-TOLIL ..... Feed flash tolerance for the inside loop. Use for reactive distillation only. (Default=$1x10^{-7}$)

PHEQM-FORM..... Phase equilibrium formulation for Newton-based methods.

PHEQM-FORM=STANDARD	Includes composition derivatives (Default)
PHEQM-FORM=TOTAL-FLOW	Includes total flow as a variable
PHEQM-FORM=IDEAL	Ignores composition derivatives

RADIUS-FRAC ..... Initial dogleg radius when using dogleg strategy to stabilize Newton's method (Default=0.1)

COL-CONFIG

Use to enter column configuration choices. These include condenser and reboiler configurations and the method for selecting key-components for column targeting analysis. If you specify the condenser configuration, you do not need to specify distillate vapor fraction (RDV) in the COL-SPECS sentence, except for partial condensers with both vapor and liquid distillates.

CONDENSER..... Condenser configuration

CONDENSER=TOTAL	Total condenser with a liquid distillate (RDV=0)
CONDENSER=PARTIAL-V	Partial condenser with vapor distillate only (RDV=1)
CONDENSER= PARTIAL-V-L	Partial condenser with vapor and liquid distillates (0< RDV<1)
CONDENSER=NONE	No condenser. Reflux is provided by an external feed or pumparound return to the top stage (condenser heat duty=0; RDV=1)

REBOILER ..... Reboiler configuration

REBOILER=KETTLE	Kettle type reboiler (Default)
REBOILER= THERMOSYPHON	Thermosyphon reboiler
REBOILER=NONE	No reboiler (reboiler heat duty=0). Boilup is provided by external feed or pumparound return to the bottom stage.

KEY-SELECT ..... Method for selection of light and heavy key components for column targeting analysis. Specify KEY-SELECT if TARGET or HYDANAL report option is chosen in the REPORT sentence.

KEY-SELECT=USER	Use specified light and heavy key components from KEY-COMP sentence.
KEY-SELECT= SPLIT-FRACTION	Select the light and heavy key components on the basis of component split-fractions in column product streams. This method is best suited for sharp or near-sharp splits.
KEY-SELECT=K-VALUE	Select the light and heavy key components on the basis of component K-values. This method is best suited for sloppy splits. (Default)
KEY-SELECT= COMP-PROFILE	Select the light and heavy key components on the basis of composition profiles. In principle, this method is similar to KEY-SELECT= K-VALUE. It is best suited for sloppy splits and it is, in general, inferior to KEY-SELECT= K-VALUE.

FEEDS

Use to enter inlet material and heat stream locations and feed conventions for material streams.

sid..... Stream ID

stage..... Stage number

feed-conv.....	**ABOVE-STAGE**	Introduces feed between stages, above designated stage (Default)
	ON-STAGE	Introduces feed on designated stage
	DECANTER	Introduces feed to decanter attached to designated stage

PRODUCTS

Use to enter outlet material and heat stream locations, phases, and flows. For material streams, you can enter a phase specification. The phase specification for the distillate must be consistent with the specified value of RDV. When RDV does not equal zero or unity, or when RDV is a manipulated variable, two distillate products are required: one vapor, one liquid. If a liquid product contains two phases, the two phases can be separated into two product streams: one with phase L1 and the other with phase L2 or W (for free-water). The flow rate of a distillate or bottoms stream is not specified in a PRODUCTS sentence, but is specified in a COL-SPECS sentence, or left as a calculated value. The flow rate of a decanter product stream is not specified in a PRODUCTS sentence, but is left as a calculated value.

sid..... Stream ID

stage..... Stage number

phase.....

L	Total liquid (Default)
V	Vapor
L1	First-liquid
L2	Second-liquid
W	Free-water
TL	Total drawoff of stage liquid
TV	Total drawoff of stage vapor

basis-FLOW..... Flow rate for side products on a MOLE, MASS, or STDVOL basis. When *phase* is TL and TV, specified values are treated as initial estimates only.

SDRAW:FEED

Use to specify the sidedraw flow rate as a ratio to the feed flow rate.

sid..... Side stream ID

ratio..... Molar ratio of sidedraw flow rate to feed flow rate $S/\Sigma\Sigma F_{ij}$

Where:

S=	Sidedraw flow rate
F=	Feed flow rate
i =	Component in the COMPS list
j =	Stream in the STREAMS list

STREAMS ..... List of feed streams forming the basis for the ratio specification. Default is all streams.

COMPS ..... List of components forming the basis for the ratio specification. Default is all components.

PSEUDO-STREAM

Use to identify outlet streams as pseudoproduct streams. A pseudostream can be a stage flow, thermosyphon reboiler flow or pumparound. Enter locations, phases, and flows for stage flows. If no flow rate specification is given, the net flow (excluding any product withdrawn) of the specified phase from the specified stage is stored in the pseudoproduct stream.

sid..... Stream ID

stage..... Stage number required for stage flows and thermosyphon reboiler flows

PHASE..... Phase specification required for stage flows and thermosyphon reboiler flows:

PHASE=L	Total liquid (Default)
PHASE=V	Vapor
PHASE=L1	First-liquid
PHASE=L2	Second-liquid

PHASE=W	Free-water
PHASE=R	Thermosyphon reboiler circulation flow
PHASE=RL	Liquid portion of thermosyphon reboiler circulation flow
PHASE=RV	Vapor portion of thermosyphon reboiler circulation flow

MOLE-FLOW ..... Molar flow rate (Default=net flow)

PA ..... Pumparound ID, required for pumparound

STATE ..... State condition for pumparound or thermosyphon reboiler circulation flow:

STATE=OUTLET	Outlet state condition is stored (Default)
STATE=INLET	Inlet state condition is stored

P-SPEC

Use to specify the column pressure profile. There are three methods for entering column pressure profile:

- Use P-SPEC to enter the pressure profile.
- Use P-SPEC to enter the top and second stage pressure. Enter pressure drop using the DP-COL and DP-STAGE keywords in the COL-SPECS sentence.
- Use P-SPEC to enter top stage pressure. Use the PDROP-SEC sentence to enter pressure drop for column sections.

stage..... Stage number

pres ..... Pressure

COL-SPECS

Use to enter the distillate vapor fraction (RDV) or top stage temperature (T1), and up to two additional column specifications. Tables 15.1 and 15.2 on pages 15-253 and 15-254 list the valid column specification combinations. When specifying top stage temperature (T1), the temperature should correspond to a vapor liquid region. If ALGORITHM=STANDARD and FREE-WATER=YES, COL-SPECS is used to enter the free-water reflux ratio (RW). You can also enter the column pressure drop, condenser pressure drop, or pressure drop per stage.

For design mode, any quantities specified in a COL-SPECS statement (except DP-STAGE, DP-COL, and DP-COND) can be treated as manipulated variables, in which case the values given in the COL-SPECS statement are initial guesses. Inlet heat streams to the top or bottom stage can be used in place of Q1 or QN. Substitute MOLE, MASS, or STDVOL for the word *basis* in the following specifications.

basis-RDV ..... Distillate vapor fraction (RDV=DV/D)
Where:
DV = Distillate vapor flow rate
D = Total distillate flow rate, excluding any free-water when NPHASE=2 and FREE-WATER=YES

You cannot enter basis-RDV if you specify T1. You do not need to specify basis-RDV when CONDENSER=TOTAL, PARTIAL-V or NONE in the COL-CONFIG sentence.

T1 ..... Condenser temperature, allowed only for partial condenser with both liquid and vapor distillate products. You cannot enter T1 if basis-RDV is specified.

basis-D ..... Total distillate flow rate, excluding any free-water when NPHASE=2 and FREE-WATER=YES

basis-B..... Bottoms flow rate

D:F..... Molar ratio of distillate flow rate to feed flow rate ($D/\Sigma\Sigma F_{ij}$)

B:F ..... Molar ratio of bottoms flow rate to feed flow rate ($B/\Sigma\Sigma F_{ij}$)

Where:
F = Feed flow rate
i = Component in the COMPS list of the DB:F-PARAMS sentence
j = Stream in the STREAMS list of the DB:F-PARAMS sentence

basis-D:F ..... Ratio of distillate flow rate to feed flow rate. Use when basis is MASS or STDVOL.

basis-B:F..... Ratio of bottoms flow rate to feed flow rate. Use when basis is MASS or STDVOL.

basis-L1 ..... Reflux flow rate (or the liquid flow rate from the top stage), excluding any free-water when NPHASE=2 and FREE-WATER=YES

basis-VN ..... Boilup flow rate (or the vapor flow rate from the bottom stage)

basis-RR ..... Reflux ratio (L1/D), excluding any free-water when NPHASE=2 and FREE-WATER=YES

basis-BR ..... Boilup ratio (VN/B)

Q1..... Condenser (or top stage) heat duty

QN ..... Reboiler (or bottom stage) heat duty

RW..... Free-water reflux ratio on a mole basis; RW=LW/DW
Where:
LW = Free-water reflux rate
DW = Free-water distillate rate
(Default=0)

DP-STAGE ..... Pressure drop per stage

DP-COL ..... Pressure drop for column

DP-COND ..... Pressure drop across condenser

HTLOSS..... Heat loss for column. A positive value of heat loss corresponds to heat flow from the tray to the surroundings. The specified value is divided equally among all stages in the column. For rate-based calculations, the heat loss is applied to the liquid phase. You cannot enter HTLOSS if you specify a HTLOSS-SEC or HTLOSS sentence.

This keyword is still supported, but it is recommended that the HTLOSS-LIQ keyword in the HTLOSS sentence be used instead of this keyword.

DB:F-PARAMS Use to define the basis for the D:F and B:F specifications in the COL-SPECS sentence.

STREAMS ..... List of feed streams forming the basis for the D:F or B:F specifications (Default=all feed streams to the block)

COMPS ..... List of components forming the basis for the D:F or B:F specifications (Default=all components)

SC-REFLUX Use to specify either the degrees subcooling of the reflux, or the reflux temperature. If you do not enter a SC-REFLUX statement, the reflux is assumed to be a saturated liquid. Subcooled reflux is not allowed when NPHASE=3. When FREE-WATER=YES, subcooled reflux is allowed only if you specify ALGORITHM=SUM-RATES and basis-RDV=0.

DEGSUB ..... Degrees subcooling

TEMP..... Reflux temperature

OPTION..... **OPTION=0** Both reflux and liquid distillate are subcooled (Default)

OPTION=1 Only reflux is subcooled

THERMOSYPHON

Use to enter pressure and up to two additional specifications for the thermosyphon reboiler. The thermosyphon reboiler model has five related variables: pressure, circulation rate, temperature, temperature change, and vapor fraction. Pressure may be specified or defaulted to the bottom stage pressure. In addition, one of the following specification options must be chosen:

1. Temperature
2. Temperature change
3. Vapor fraction
4. Circulation flow
5. Circulation flow and temperature
6. Circulation flow and temperature change
7. Circulation flow and vapor fraction

Options 5 through 7 are not allowed when NPHASE=3. If options 1 through 4 are chosen, the duty QN is either specified or left as a calculated value. If option 5, 6 or 7 is specified, QN must be specified in the COL-SPECS sentence, but is treated as an initial guess.

If no THERMOSYPHON statement is given, the reboiler is assumed to be of the kettle type.

PRES ..... Reboiler pressure (Default=bottom stage pressure)

TEMP ..... Temperature of reboiler outlet

DELT ..... Temperature change across reboiler

VFRAC ..... Vapor fraction of reboiler outlet

basis-FLOW ..... Circulation flow on a MOLE, MASS, or STDVOL basis

RETURN-CONV ..... Convention for returning reboiler outlet to column:

RETURN-CONV= ABOVE-STAGE	Introduces reboiler outlet between Nstage and Nstage–1, with vapor portion going to Nstage–1 and liquid going to Nstage
RETURN-CONV= ON-STAGE	Introduces reboiler outlet to Nstage (Default)

PUMPAROUND

Use to enter pumparound connectivity and heater/cooler specifications. Pumparounds can be total or partial drawoffs of the stage flow. You must specify the source, and return stage locations for each pumparound. By default RADFRAC assumes the pumparound does not experience any phase change at the heater/cooler outlet. However, you can specify NPHASE=2 or 3, and let RADFRAC determine the return phase condition from the heater/cooler specifications.

paid ..... Pumparound ID

stage1 ..... Source stage number

stage2 ..... Destination stage number

DRAW-PHASE ..... Phase of pumparound stream at the source:

L	Liquid (Default)
L1	First-liquid
L2	Second-liquid
V	Vapor

TYPE ..... Pumparound drawoff type:

TYPE=PARTIAL	Partial drawoff. You must specify two of the following variables: basis-FLOW, DUTY, TEMP (or DELT), or VFRAC. (Default)

	TYPE=TOTAL	Total drawoff. You must specify one of the following variables: TEMP, DELT, VFRAC or DUTY.

basis-FLOW..... Pumparound flow rate in MOLE, MASS, or STDVOL basis

TEMP..... Temperature of pumparound stream at associated heater/cooler outlet

DELT ..... Change in temperature of pumparound stream across associated heater/cooler outlet

DUTY..... Heat duty for associated heater/cooler. Enter a negative value for cooling, a positive value for heating, and 0 for no heating or cooling.

VFRAC..... Vapor fraction of pumparound stream at associated heater/cooler outlet. VFRAC is not allowed when NPHASE=1.

PRES..... Pressure of pumparound stream at associated heater/cooler outlet (Default=pressure of draw stage)

NPHASE ..... Number of phases at the associated heater/cooler outlet (Default=1)

RETURN-PHASE..... Phase of pumparound stream at associated heater/cooler outlet when NPHASE=1: L or V

FEED-CONV ..... Feed convention for returning pumparound to column:

FEED-CONV= ABOVE-STAGE	Introduces pumparound above designated stage
FEED-CONV=ON-STAGE	Introduces pumparound to designated stage (Default)
FEED-CONV=DECANTER	Introduces pumparound to decanter attached to designated stage

QSTREAM-IN..... Stream ID of inlet heat stream for the pumparound

QSTREAM-OUT ..... Stream ID of outlet heat stream for the pumparound

HEATERS

Use to enter the heater stage locations and duties. Inlet heat streams can be used in place of HEATERS specifications.

stage..... Stage number

duty ..... Heat duty

COOLANT

Use to define interstage heaters/coolers with UA and coolant specifications. You must specify the UA and the coolant component, flow rate and inlet temperature. You can specify the heat capacity directly, or RADFRAC calculates it from a coolant property option set. If the heat capacity is to be calculated, you must enter the pressure and phase of the coolant. UA calculations assume that no phase change occurs on the coolant side.

stage..... Stage number

cid..... Component ID

opsetname..... Property option set name (Default=property option set for corresponding stage)

basis-FLOW..... Coolant flow rate in MOLE, MASS or STDVOL basis

UA..... Product of the average heat-transfer coefficient and heat-transfer area

TEMP..... Coolant inlet temperature

PRES..... Coolant pressure

PHASE..... Phase of coolant, L or V

basis-CP..... Average heat capacity for coolant in MOLE, MASS, or STDVOL basis. The basis should be the same as the basis for the coolant flow rate.

HTLOSS-SEC Heat loss for a section of the column, by phase. Heat loss may only be specified by one of the HTLOSS-SEC sentence, the HTLOSS sentence, or the HTLOSS keyword in the COL-SPECS sentence.

secno..... Section number

stage1..... Stage number for initial stage of column segment

stage2..... Stage number for final stage of column segment

heat loss..... Heat loss for the column section. A positive value of heat loss corresponds to heat flow from the tray to the surroundings. The specified value is divided equally among stages in the column section.

HTLOSS-SEC..... Heat loss for the liquid phase in the section. Enter a positive value for the heat loss, which is split uniformly over the stages in the section.

HTLOSS-VAP..... Heat loss for the vapor phase in the section. Enter a positive value for the heat loss, which is split uniformly over the stages in the section.

In equilibrium calculations, the heat losses specified for HTLOSS-SEC and HTLOSS-VAP are combined and applied to the stage as a whole.

HTLOSS Heat loss for the entire column, by phase. Heat loss may only be specified by one of the HTLOSS-SEC sentence, the HTLOSS sentence, or the HTLOSS keyword in the COL-SPECS sentence.

HTLOSS-LIQ..... Heat loss for the liquid phase. Enter a positive value for the heat loss, which is split uniformly over the stages in the column.

HTLOSS-VAP..... Heat loss for the vapor phase. Enter a positive value for the heat loss, which is split uniformly over the stages in the column.

In equilibrium calculations, the heat losses specified for HTLOSS-LIQ and HTLOSS-VAP are combined and applied to the stage as a whole.

COMP-EFF Use to enter component efficiencies. The type of efficiency is specified by EFF in the PARAM statement. When NPHASE=3, COMP-EFF applies to both liquid phases. You cannot use COMP-EFF if you specify STAGE-EFF, STAGE-EFF-SEC, L1-COMP-EFF, L2-COMP-EFF, L1-STAGE-EFF, or L2-STAGE-EFF.

stage..... Stage number

cid..... Component ID

eff..... Efficiency (Default=1)

STAGE-EFF Use to enter stage efficiencies. These efficiencies are applied to each component on the stage. The type of efficiency is specified by EFF in the PARAM statement. When NPHASE=3, STAGE-EFF applies to both liquid phases. You cannot use STAGE-EFF if you specify STAGE-EFF-SEC, COMP-EFF, L1-COMP-EFF, L2-COMP-EFF, L1-STAGE-EFF, or L2-STAGE-EFF.

stage..... Stage number

eff..... Efficiency (Default=1)

STEFF-SEC

Use to enter stage efficiencies for a column section. These efficiencies are applied to each component on each stage in the column section. The type of efficiency is specified by EFF in the PARAM sentence. When NPHASE=3, STEFF-SEC applies to both liquid phases. You cannot use STEFF-SEC if you specify COMP-EFF, STAGE-EFF, L1-COMP-EFF, L2-COMP-EFF, L1-STAGE-EFF, or L2-STAGE-EFF.

secno ..... Section number

stage1..... Stage number for initial stage of column segment

stage2..... Stage number for final stage of column segment

eff..... Efficiency (Default=1)

DECANTERS

Use to enter location and other specifications for decanters when NPHASE=3. For the top stage decanter you must specify the fraction of at least one of the two phases returned. For all other decanters, you must specify the fraction of each of the two liquid phases returned. You can specify temperature or degrees of subcooling.

stage..... Stage number

L1-SPEC..... Fraction of the first-liquid phase returned

L2-SPEC..... Fraction of the second-liquid phase returned

TEMP..... Temperature of decanter (Default=stage temperature)

DEGSUB ..... Degrees subcooling (Default=0)

DECANT-SOLID ..... Solids decant option:

DECANT-SOLID=PARTIAL	Decant solids partially using L2-SPEC as the solid return fraction (Default)
DECANT-SOLID=TOTAL	Decant solids completely

NQ-CURVE

Use to enter NQ-curve specifications. Enter one NQ-CURVE sentence for each NQ-CURVE specification.

CURVE-NO..... NQ curve number

NSTAGE-MIN..... Lower limit on number of stages

NSTAGE-MAX ..... Upper limit on number of stages

NSTAGE-STEP ..... Step size for number of stages (Default = 2)

FEED ..... ID of the sampled feed stream. The total number of stages and the location of this feed stream will be optimized.

RR-MIN..... Minimum reflux ratio (Default = 1E-6)

OBJECT-FUNC..... Objective function for optimizing total number of stages and feed stream location:

OBJECT-FUNC= QREB-QCOND	Total heat load of condenser and reboiler (Default)
OBJECT-FUNC= QCOND	Condenser heat load (absolute value)
OBJECT-FUNC= QREB	Reboiler heat load
OBJECT-FUNC= MOLE-RR	Molar reflux ratio
OBJECT-FUNC= MASS-RR	Mass reflux ratio
OBJECT-FUNC= STDVOL-RR	Standard liquid volume reflux ratio

LMT-FROM-TOP..... Limit on feed stage location from the top (Default = 1)

LMT-FROM-BOT..... Limit on feed stage location from the bottom (Default = 1)

QR-QC-COST ..... Reboiler / condenser cost ratio. Used when OBJECT-FUNC = QREB-QCOND.

NQCUR-FOPT Use to enter options to vary locations of material feeds other than the sampled one in the corresponding NQ-CURVE sentence. These material feeds are also referred to as "remaining feed streams." REL-FEED is assumed for unspecified streams.

CURVE-NO..... NQ curve number

SID ..... Feed stream ID. Only remaining feed streams can be specified.

REMAIN-OPT..... Method for varying remaining feed stream location:

REMAIN-OPT= REL-FEED	Maintain proportional location between the sampled feed and end of column (Default)
REMAIN-OPT= RELATIVE	Maintain proportional location within the entire column
REMAIN-OPT= FROM-TOP	Maintain absolute number of stages from top
REMAIN-OPT= FROM-BOTTOM	Maintain absolute number of stages from bottom
REMAIN-OPT= FROM-FEED	Maintain absolute number of stages above or below sampled feed

NQCUR-SOPT Use to enter options to vary locations of side-draws. REL-FEED is assumed for unspecified side-draws.

CURVE-NO..... NQ curve number

SID ..... Side-draw product stream ID

SDRAW-OPT..... Method for varying side-draw location:

SDRAW-OPT= REL-FEED	Maintain proportional location between the sampled feed and end of column (Default)
SDRAW-OPT= RELATIVE	Maintain proportional location within the entire column
SDRAW-OPT= FROM-TOP	Maintain absolute number of stages from top
SDRAW-OPT= FROM-BOTTOM	Maintain absolute number of stages from bottom
SDRAW-OPT= FROM-FEED	Maintain absolute number of stages above or below sampled feed

NQCUR-PAOPT Use to enter options to vary locations of pumparounds. REL-FEED is assumed for unspecified pumparounds.

CURVE-NO..... NQ curve number

IC-STREAM ..... Pumparound ID

PA-OPT ..... Method for varying pumparound location:

PA-OPT= REL-FEED	Maintain proportional location between the sampled feed and end of column (Default)
PA-OPT= RELATIVE	Maintain proportional location within the entire column
PA-OPT= FROM-TOP	Maintain absolute number of stages from top
PA-OPT= FROM-BOTTOM	Maintain absolute number of stages from bottom
PA-OPT= FROM-FEED	Maintain absolute number of stages above or below sampled feed

NQCUR-DECTOP Use to enter options to vary locations of decanters. REL-FEED is assumed for unspecified decanters.

CURVE-NO..... NQ curve number

STAGE..... Decanter stage number

DECT-OPT ..... Method for varying decanter location:

DECT-OPT= REL-FEED	Maintain proportional location between the sampled feed and end of column (Default)

DECT-OPT= RELATIVE	Maintain proportional location within the entire column
DECT-OPT= FROM-TOP	Maintain absolute number of stages from top
DECT-OPT= FROM-BOTTOM	Maintain absolute number of stages from bottom
DECT-OPT= FROM-FEED	Maintain absolute number of stages above or below sampled feed

L2-COMPS Use to enter a list of key components that are used to identify the second-liquid phase when NPHASE=3 and FREE-WATER=NO. The liquid phase with the larger mole fraction of the key components is designated as the second-liquid phase. If NPHASE=3 and FREE-WATER=YES, the free-water phase is the second-liquid phase.

cid-list ..... Key component ID list

L2-STAGES Use to indicate a segment of stages to be tested for the presence of two liquid phases when NPHASE=3.

stage1..... Stage number for initial stage of column segment

stage2..... Stage number for final stage of column segment. If the segment to be tested consists only of *stage1*, enter an asterisk for *stage2*.

L1-RETURN Use to enter optional decanter return specifications for the first-liquid phase. You can split the first-liquid phase into any number of streams, each of which goes to a different stage. If you do not specify L1-RETURN, the first-liquid phase is returned to the stage immediately below the decanter stage.

stage1..... Stage number of decanter

stage2..... Stage number of stage to which the first-liquid phase of decanter is returned

l1-rfrac ..... Fraction of decanter liquid1 returned to the return stage

L2-RETURN Use to enter optional decanter return specifications for the second-liquid phase. You can split the second-liquid phase into any number of streams, each of which goes to a different stage. If you do not specify L2-RETURN, the second-liquid phase is returned to the stage immediately below the decanter stage.

stage1..... Stage number of decanter

stage2..... Stage number of stage to which the second-liquid phase of decanter is returned

l2-rfrac ..... Fraction of decanter liquid2 returned to the return stage

L1-COMP-EFF Use to enter component Murphree or vaporization efficiencies for the first-liquid phase when NPHASE=3. The type of efficiency is specified by EFF in the PARAM statement. You cannot use L1-COMP-EFF if you specified L1-STAGE-EFF, L2-STAGE-EFF, STAGE-EFF, STAGE-EFF-SEC, or COMP-EFF.

stage..... Stage number

cid..... Component ID

eff..... Efficiency (Default=1)

L2-COMP-EFF Use to enter component Murphree or vaporization efficiencies for the second-liquid phase when NPHASE=3. The efficiency type is specified by EFF in the PARAM statement. You cannot use L2-COMP-EFF if you specified L1-STAGE-EFF, L2-STAGE-EFF, STAGE-EFF, STAGE-EFF-SEC, or COMP-EFF.

stage..... Stage number

cid..... Component ID

eff..... Efficiency (Default=1)

L1-STAGE-EFF Use to enter component Murphree or vaporization efficiencies for the first-liquid phase when NPHASE=3. These efficiencies are applied to each component on the stage. The efficiency type is specified by EFF in the PARAM statement. You cannot use L1-STAGE-EFF if you specified L1-COMP-EFF, L2-COMP-EFF, STAGE-EFF or COMP-EFF.

stage..... Stage number

eff..... Efficiency (Default=1)

L2-STAGE-EFF Use to enter component Murphree or vaporization efficiencies for the second-liquid phase when NPHASE=3. These efficiencies are applied to each component on the stage. The efficiency type is specified by EFF in the PARAM statement. You cannot use L2-STAGE-EFF if you specified L1-COMP-EFF, L2-COMP-EFF, STAGE-EFF or COMP-EFF.

stage..... Stage number

eff..... Efficiency (Default=1)

KLL-STAGES Use to specify column segment for which the built-in KLL expression is used. You must also specify basis-KLL and NPHASE=3.

kll-no..... KLL dataset number

stage1..... Initial stage of a column segment

stage2..... Final stage of a column segment

basis-KLL Use to enter coefficients in MOLE, MASS, or STDVOL basis for the built-in KLL expression. You must also specify NPHASE=3.

KLL-NO..... KLL dataset number

KLL-CID..... Component ID

KLL-A, KLL-B..... Coefficients for KLL expression. Which is defined as:
KLL-C, KLL-D

$$\ln(KLL) = (KLL\text{-}A) + (KLL\text{-}B)/T + (KLL\text{-}C) \times \ln T + (KLL\text{-}D) \times T$$

Where:
KLL = Liquid-liquid equilibrium K-value
T = Temperature in Kelvin

You must enter a value for KLL-A. The default values for the other coefficients are zero.

REAC-STAGES Use to specify the set of chemical reactions occurring in a segment of stages.

stage1..... Stage number for initial stage of column segment

stage2..... Stage number for final stage of column segment. If the segment consists only of *stage1*, enter an asterisk for *stage2*.

reactid..... REACTIONS or CHEMISTRY paragraph ID. RADFRAC accepts only REACTIONS types REAC-DIST and USER. (See Chapters 5 and 6.)

HOLD-UP Use to specify liquid and/or vapor holdup for segment(s) of columns in which rate-controlled reactions occur. You cannot use HOLD-UP if you specified RES-TIME. Substitute MOLE, MASS, or VOL for the word *basis* in the following specifications.

stage1..... Stage number for initial stage of column segment

stage2..... Stage number for final stage of column segment. If the segment consists only of *stage1*, enter an asterisk for *stage2*.

basis-LHLDP..... Liquid holdup

basis-VHLDP..... Vapor holdup

RES-TIME Use to specify residence time in the liquid and/or vapor phase for segment(s) of columns in which rate-controlled reactions occur. You cannot use RES-TIME if you specified HOLD-UP.

stage1..... Stage number for initial stage of column segment

stage2..... Stage number for final stage of column segment. If the segment consists only of *stage1*, enter an asterisk for *stage2*.

LTIME ..... Residence time in liquid phase

VTIME ..... Residence time in vapor phase

CONVERSION Use to override fractional conversion for reactions (based on key components) specified in the REACTIONS paragraph. (See Chapter 6.)

stage..... Stage number

reacno ..... Reaction number in REACTIONS paragraph

frac ..... Fractional conversion based on key component

T-EST Use to enter an initial estimate of the column temperature profile. If you do not enter a T-EST sentence, an initial profile is generated by RADFRAC.

stage..... Stage number

temp ..... Temperature

X-EST, Y-EST Use to enter an initial estimate of the column composition profiles. X-EST and Y-EST are always used together.

stage..... Stage number

cid..... Component ID

x ..... Liquid mole fraction for total liquid phase

y ..... Vapor mole fraction

L-EST, V-EST, VL-EST Use to enter initial flow or flow ratio estimates for the liquid phase (L-EST), vapor phase (V-EST), and the ratio of vapor to liquid (VL-EST) when ABSORBER=YES or ALGORITHM=SUM-RATES. You cannot use L-EST (or V-EST), and VL-EST together. The flows or flow ratios entered refer to the net flow on a stage, excluding any side product withdrawn.

stage..... Stage number

mole-flow ..... Molar flow rate (for L-EST or V-EST)

mole-ratio..... Ratio of vapor mole flow to liquid mole flow (for VL-EST)

REPORT Use to override the default report options. You can use the standard REPORT options for use within a block (see Chapter 11) for RADFRAC.

reportopt ..... Standard block report options (see Chapter 11), in addition to the following:

NOPROFILE	Suppress the stagewise profiles of temperature, operating pressure, flows, enthalpies, and duties for this block
NOCOMPS	Suppress the mole fraction and K-value profiles for this block
NOHYDRAULIC	Suppress the hydraulic parameters reported for this block
NOENTH	Suppress the enthalpy profile for this block
NOSPLITS	Suppress the summary of component split fractions among product streams for this block
STDVPROF	Include stagewise profiles of standard volume flows for this block in column profiles.
TARGET	Include column targeting thermal analysis results

HYDANAL	Include column targeting hydraulic analysis results
EXTHYD	Include extended hydraulic parameter report. Use only when NOHYDRAULIC report option is not selected or when HYDRAULIC=YES in the PARAM sentence.

The additional report options below apply only to RateSep rate-based distillation calculations:

INT-PROF	Include interfacial fractions, temperatures and K-value.
INT-AREA	Include interfacial area.
BULKRXN	Include bulk reaction rates.
DIFF-COE	Include binary diffusion coefficients.
MT-RATE	Include mass transfer rates.
MT-COEFF	Include binary mass transfer coefficients.
HT-RATE	Include heat transfer rates.
HT-COEFF	Include heat transfer coefficients.
FILMRXN	Include reaction rates within films.
S-DIMLES	Include scalar dimensionless numbers.
V-DIMLES	Include Schmidt and Sherwood numbers.

SPC-OPTIONS Use to specify additional stage and design-spec variables to include or exclude in EO calculations. All options can be set to YES or NO. (Default=YES; these variables are included in EO calculations unless specified otherwise.)

EFF	Whether to include additional efficiency variable
D	Whether to include additional distillate variable
B	Whether to include additional bottom flow variable
RR	Whether to include additional reflux ratio variable
L1	Whether to include additional reflux rate variable
BR	Whether to include additional boilup ratio variable
VN	Whether to include additional boilup rate variable
Q1	Whether to include additional condenser duty variable
QN	Whether to include additional reboiler duty variable
L	Whether to include additional liquid flow variable
V	Whether to include additional vapor flow variable
Q-STAGE	Whether to include additional stage duty variable
WL	Whether to include additional liquid side-draw variable
WV	Whether to include additional vapor side-draw variable
SPEC	Whether to include additional design specification variables
SC-REFLUX	Whether to include additional reflux sub-cooling variable

SPC-OPTION2 Use to specify additional features to include or exclude in EO calculations. All options can be set to YES or NO. (Default=YES)

PRES	Whether to include pressure and pressure drops for all stages
FEEDDP	Whether to include feed-to-stage pressure drop
FEEDOPEN	Option for open feed flash. Do not specify when NPHASE=3.

CS-ALLBASIS ..... Whether to include flow rate and ratio specifications in all flow basis (MOLE, MASS, and STDVOL)

SPLIT-ALL..... Whether to include second liquid or free-water variables for all stages that are tested for two liquid phases (Default=NO). Do not specify when NPHASE=2.

KEY-COMP Use to specify light and heavy key components for column targeting analysis. Use only when TARGET and/or HYDANAL report option is selected and KEY-SELECT=USER in the COL-CONFIG sentence.

secno ..... Section number for key component specification

stage1..... Stage number for the initial stage of the section

stage2..... Stage number for the final stage of the section

LIGHT-KEY..... List of light key components

HEAVY-KEY ..... List of heavy key components

KEY-TOL Use to specify tolerances and other parameters for light and heavy key component selection methods other than KEY-SELECT=USER and for exergy loss calculations. Use only when TARGET and/or HYDANAL report option is selected.

KVAL-TOL..... Tolerance on component K-values. Specify when KEY-SELECT= K-VALUE or SPLIT-FRACTION. (Default=$1x10^{-5}$)

COMP-TOL..... Tolerance on component mole-fractions. Specify when KEY-SELECT=
K-VALUE, SPLIT-FRACTION, or COMP-PROFILE. (Default=$1x10^{-6}$)

SPF-LIMIT..... Minimum value of component split-fractions, in the top and the bottom products of a column section, necessary for key component selection. Specify when KEY-SELECT=SPLIT-FRACTION. (Default=0.9)

STG-SPAN ..... Stage span for computing composition profiles. Specify when KEY-SELECT=COMP-PROFILE. (Default=2)

EXCLD-KEY..... List of components to be excluded from key component selection. Specify when KEY-SELECT=K-VALUE, SPLIT-FRACTION, or COMP-PROFILE.

EXG-TREF..... Reference temperature for exergy loss calculations (Default=298.15 K)

CONVERGENCE Use to specify advanced convergence parameters.

MAN-3P-PASS ..... Number of initialization passes in which two liquid phases are forced to be present. Should not exceed 8. (Default=0)

STABLE-ITER ..... Initial number of iterations over which the steps are damped using a stabilization method. Use when ALGORITHM=NEWTON or when ILMETH=NEWTON in the PARAM sentence.

STABLE-METH ..... Stabilization method. Use when ALGORITHM=NEWTON or when ILMETH=NEWTON in the PARAM sentence.

STABLE-METH=DOGLEG	Powell's dogleg strategy (Default)
STABLE-METH= LINE-SEARCH	One-dimensional line search

PROP-DERIV ..... Property derivative calculation method for ALGORITHM=NEWTON.

PROP-DERIV= ANALYTICAL	Analytical (Default)
PROP-DERIV=NUMERICAL	Numerical

NQ-PROF-MAX ..... Maximum number of NQ profiles stored for analysis (Default=original number of stages * number of NQ curves)

NQ-FOPT-METH ..... Algorithm for feed tray optimization.

NQ-FOPT-METH= CASE-STUDY	Feed tray optimization by case study
NQ-FOPT-METH=QP-SRCH	Feed tray optimization by one-dimensional quadratic search
NQ-FOPT-METH=HYBRID	Feed tray optimization by one-dimensional quadratic search for first case and by case study for subsequent cases (Default)

NQ-TOLOL ..... Outside loop tolerance used during NQ curve generation. (Default=10^{-5})

NQ-TOLOBJ ..... Objective function tolerance for terminating NQ curve generation. Generation terminates when the variation of objective function when increasing the number of stages by 1 falls below this tolerance. (Default=0.01)

TRAY-REPORT Use to specify the format of the report and additional tray properties to be reported (in addition to the flows, temperatures, pressures, enthalpies, duties, mole fractions, and K-values printed in the standard report).

TRAY-OPTION ..... Specifies stages included in the report:

TRAY-OPTION=BRIEF	Reports the stages that have feeds, products, heaters, and maximum and minimum flows, and the stages immediately above and below those stages (Default)
TRAY-OPTION= INCL-TRAYS	Reports the stages specified in the INCL-TRAYS statement
TRAY-OPTION= ALL-TRAYS	Reports all stages

FORMAT .....

FORMAT=PROFILE	Prints tabular column profiles (Default)
FORMAT=STAGE	Prints individual stage reports
FORMAT=COMBINED	Prints both tabular column profiles and individual stage reports

ORDER ..... Tray numbering order. Use for report only.

ORDER=TOP-DOWN	Numbers stages from top down (Default)
ORDER=BOTTOM-UP	Numbers stages from bottom up

PROPERTIES ..... List of property set Ids

WIDE ..... Report width option

WIDE=YES	Produce wide (132 columns) reports (Default)
WIDE=NO	Produce standard (80 columns) reports

TRAY-REPOPT Use to specify the flow profile option for the block report.

FLOW-OPTION .....

FLOW-OPTION=0	Report flows from a stage including side draws, side products, and pumparounds (Default)
FLOW-OPTION=1	Report flows from a stage excluding side draws, side products, and pumparounds

INCL-TRAYS Use to designate stages to be included in the report when TRAY-OPTION=INCL-TRAYS in the TRAY-REPORT sentence.

stage1..... Stage number of initial stage of column segment to be reported

stage2..... Stage number of final stage of column segment to be reported (Default=*stage1*)

COND-HCURVE Use to generate cooling curve tables for the condenser. If you entered efficiency or reaction specification for the condenser using COMP-EFF, STAGE-EFF, L1-COMP-EFF, L2-COMP-EFF, L1-STAGE-EFF, L2-STAGE-EFF, or REAC-STAGES, condenser cooling curves will not be consistent with column results. See Chapter 11 for a description of input keywords.

REB-HCURVE Use to generate heating curve tables for the reboiler. If you entered efficiency or reaction specification for the reboiler using COMP-EFF, STAGE-EFF, L1-COMP-EFF, L2-COMP-EFF, L1-STAGE-EFF, L2-STAGE-EFF, or REAC-STAGES, reboiler heating curves will not be consistent with column results. See Chapter 11 for a description of input keywords.

PA-HCURVE Use to generate heating/cooling curve tables and plots for pumparound heater/cooler. You must specify the pumparound ID. See Chapter 11 for a description of input keywords.

paid ..... Pumparound ID

VARY Use to specify manipulated variables for the design mode. FEED-FLOW and HEAT-STREAM are initialized in a STREAM paragraph. You must enter initial guesses of the manipulated variables. For other manipulated variables, enter estimates using the usual rating mode specification keywords:

Sentence	Variables
PRODUCTS	basis-LPROD, basis-VPROD
HEATERS	DUTY
PUMPAROUND	basis-PA-FLOW, PA-TEMP, PA-DELT, PA-DUTY, PA-VFRAC
COMP-EFF or STAGE-EFF	MURPHREE
THERMOSYPHON	TREB, DTREB, VREB, basis-RFLOW
DECANTERS	L1-SPEC, L2-SPEC
COL-SPECS	All others

The initial guesses must be bracketed by the bounds *lb* and *ub*. One VARY sentence is entered for each manipulated variable. Substitute MOLE, MASS, or STDVOL for the word *basis*.

varyno ..... Manipulated variable number

vartype ..... Manipulated variable type:

basis-RDV Distillate vapor fraction (RDV=DV/D where DV is the distillate vapor flow rate and D is the total distillate flow rate, excluding any free-water when NPHASE=2 and FREE-WATER=YES)

basis-D Total distillate flow rate, excluding any free-water when NPHASE=2 and FREE-WATER=YES

basis-B Bottoms flow rate

D:F Molar ratio of distillate flow rate to feed flow rate ($D/\Sigma\Sigma F_{ij}$)

B:F Molar ratio of bottoms flow rate to feed flow rate ($B/\Sigma\Sigma F_{ij}$)

Where:
F = Feed flow rate
i = Component in the COMPS list of the DB:F-PARAMS sentence
j = Stream in the STREAMS list of the DB:F-PARAMS sentence

basis-D:F Ratio of distillate flow rate to feed flow rate. Use when basis is MASS or STDVOL.

basis-B:F Ratio of bottoms flow rate to feed flow rate. Use when basis is MASS or STDVOL.

basis-L1	Reflux flow rate (or the liquid flow rate from the top stage), excluding any free-water when NPHASE=2 and FREE-WATER=YES
basis-VN	Boilup flow rate (or the vapor flow rate from the bottom stage)
basis-RR	Reflux ratio (L1/D), excluding any free-water when NPHASE=2 and FREE-WATER=YES
basis-BR	Boilup ratio (VN/B)
Q1	Condenser (or top stage) heat duty
QN	Reboiler (or bottom stage) heat duty
RW	Free-water reflux ratio on a mole basis (RW=LW/DW) Where: LW = Free-water reflux rate DW = Free-water distillate rate
basis-LPROD	Liquid sidestream product flow from a stage (specified by STAGE)
basis-VPROD	Vapor sidestream product flow from a stage (specified by STAGE)
DUTY	External heater duty of a stage (specified by STAGE)
FEED-FLOW	Molar flow rate of a feed stream (specified by STREAM)
HEAT-STREAM	Duty of an inlet heat stream (specified by STREAM)
MURPHREE	Murphree efficiency of a group of components (specified by COMPS) in a column segment (specified by STAGE1 and STAGE2). Initial guess for Murphree efficiency must be the same for all components and for all stages in the column segment.
TREB	Thermosyphon reboiler outlet temperature
DTREB	Temperature change across thermosyphon reboiler
VREB	Thermosyphon reboiler outlet vapor fraction
basis-RFLOW	Thermosyphon reboiler circulation flow rate
L1-SPEC	Fraction of first-liquid phase returned from decanter (specified by STAGE)
L2-SPEC	Fraction of second-liquid phase returned from decanter (specified by STAGE)
basis-PA-FLOW	Circulation flow of a pumparound (specified by PA)
PA-TEMP	Temperature of a pumparound (specified by PA) at the heater/cooler outlet
PA-DELT	Temperature change across the heater/cooler of a pumparound (specified by PA)
PA-DUTY	Duty of the heater/cooler for a pumparound (specified by PA)
PA-VFRAC	Vapor fraction of a pumparound (specified by PA) at the heater/cooler outlet
SDRAW:FEED	Molar ratio of sidedraw flow rate to feed flow rate

lb ..... Lower bound

ub ..... Upper bound

step ..... Maximum step size (Default=0.1*(ub – lb))

STAGE ..... Stage number (required for *vartypes* LPROD, VPROD, DUTY, L1-SPEC, and L2-SPEC)

STREAM ..... Stream ID (required for *vartypes* FEED-FLOW, SDRAW:FEED, and HEAT-STREAM)

STAGE1 ..... Stage number for initial stage of column segment (required for *vartype* MURPHREE)

STAGE2 ..... Stage number for final stage of column segment (required for *vartype* MURPHREE)

COMPS ..... List of component IDs (required for *vartype* MURPHREE and SDRAW:FEED) (Default=all components)

PA ..... Pumparound ID (required for *vartypes* PA-FLOW, PA-TEMP, PA-DELT, PA-DUTY, and PA-VFRAC)

SPEC

Use to enter design specifications. Enter one SPEC sentence for each design specification. Substitute MOLE, MASS, or STDVOL for the word *basis*.

specno ..... Design specification number

spectype ..... Design specification type:

basis-FRAC Purity of a product stream (specified by STREAMS), an internal stream (specified by STAGE and PHASE), or a decanter stream (specified by STAGE, DEC-STREAM, and PHASE).
FRAC = $\Sigma x_i / \Sigma x_j$

Where:
x = Component fraction
i = Component in the COMPS list
j = Component in the BASE-COMPS list

The default for BASE-COMPS is all components (Σx_j=1).

basis-RECOV Component recovery.
RECOV = $\Sigma\Sigma f_{ij} / \Sigma\Sigma f_{ik}$

Where:
f = Component flow rate
i = Component in the COMPS list
j = Product stream in the STREAMS list
k = Feed stream in the BASE-STREAMS list

The default for BASE-STREAMS is all feed streams.

basis-FLOW Flow rate of a group of components (specified by COMPS) in a set of product streams (specified by STREAMS), an internal stream (specified by STAGE and PHASE), or a decanter stream (specified by STAGE, DEC-STREAM, and PHASE). The default for COMPS is all components.

basis-RATIO RATIO = $\Sigma f_{i1} / \Sigma f_{j2}$ (BASE-STAGE specified)
or
$\Sigma f_{i1} / \Sigma\Sigma f_{jk}$ (BASE-STREAMS specified or defaulted)

For basis-RATIO:

i = Component in the COMPS list

j = Component in the BASE-COMPS list

k = Stream in the BASE-STREAMS list

f_{i1}= Component *i* flow rate in an internal stream specified by STAGE and PHASE

f_{j2}= Component *j* flow rate in an internal stream specified by BASE-STAGE and BASE-PHASE

f_{jk}= Component *j* flow rate in a feed or product stream in the BASE-STREAMS list. (The BASE-STREAMS list cannot mix feed and product streams.)

The default for COMPS and BASE-COMPS is all components. The default for BASE-STREAMS is all feed streams.

TEMP	Temperature on a given STAGE
PROP	Property value, as specified by PROPERTY, for a product stream (specified by STREAMS) or an internal stream (specified by STAGE and the property phase qualifier in the corresponding PROP-SET paragraph)
PROP-DIFF	Property value minus base property value, as specified by PROPERTY and BASE-PROPERTY. PROPERTY is the property of a product stream (specified by STREAMS) or of an internal stream (specified by STAGE and the phase qualifier in the corresponding PROP-SET paragraph). BASE-PROPERTY is the property of a product stream (specified by BASE-STREAMS) or of an internal stream (specified by BASE-STAGE and the phase qualifier in the corresponding PROP-SET paragraph).
PROP-RATIO	Ratio of property value to base property value, as specified by PROPERTY and BASE-PROPERTY. PROPERTY and BASE-PROPERTY are as defined above for PROP-DIFF.
basis-D	Total distillate flow rate, excluding any free-water when NPHASE=2 and FREE-WATER=YES
basis-B	Bottoms flow rate
basis-L1	Reflux flow rate (or the liquid flow rate from the top stage), excluding any free-water when NPHASE=2 and FREE-WATER=YES
basis-VN	Boilup flow rate (or the vapor flow rate from the bottom stage)
basis-RR	Reflux ratio (L1/D), excluding any free-water when NPHASE=2 and FREE-WATER=YES
basis-BR	Boilup ratio (VN/B)
Q1	Condenser (or top stage) heat duty
QN	Reboiler (or bottom stage) heat duty

value..... Desired value of the design specification

scale ..... Scale factor (Default=1)

weight ..... Weighting factor (Default=1)

STAGE..... Stage number

BASE-STAGE ..... Stage number

COMPS ..... List of component IDs

BASE-COMPS..... List of component IDs

STREAMS ..... List of stream IDs

BASE-STREAMS ..... List of stream IDs

PROPERTY ..... ID of a property set defined by a PROP-SET paragraph consisting of a single scalar property. (See Chapter 41.)

BASE-PROPERTY ..... ID of a property set defined by a PROP-SET paragraph consisting of a single scalar property. (See Chapter 41.)

DEC-STREAM ..... **DEC-STREAM=FEED** Decanter feed

DEC-STREAM=PRODUCT Decanter product

DEC-STREAM=RETURN Decanter return

You must also specify PHASE=L and decanter stage location.

PHASE ..... **PHASE=L** Liquid (Default)

PHASE=V Vapor

PHASE=L1 First-liquid

PHASE=L2 Second-liquid

PHASE=W Free-water

BASE-PHASE ..... **BASE-PHASE=L** Liquid

BASE-PHASE=V Vapor

BASE-PHASE=L1 First-liquid

BASE-PHASE=L2 Second-liquid

BASE-PHASE=W Free-water

(Default=value specified for PHASE)

PDROP-SEC

Use to enter pressure drop across a section of a column. You must also specify the pressure for *stage1* in the P-SPEC sentence. You cannot use PDROP-SEC if you specify DP-STAGE, DP-COND, DP-COL, or P-SPEC.

secno ..... Section number

stage1 ..... Stage number for initial stage of column segment

stage2 ..... Stage number for final stage of column segment

pdrop ..... Pressure drop across section

DIAGNOSTICS

Use to control the level of convergence diagnostics in the history and log files. You can enter a level between 0 and 10. The amount of diagnostics increases with each level.

MAIN ..... Controls printouts of initial/final profiles, inside/middle/outside loop iterations, and outside loop variables/functions in the history file (Default=4)

OLVAR1 ..... Controls initial local model parameter diagnostics in the history file (Default=4)

OLVAR2 ..... Controls local model parameter diagnostics for each outside loop in the history file (Default=4)

CMBAL ..... Controls component mass balance diagnostics for each inside loop in the history file (Default=4)

EMBAL ..... Controls enthalpy balance diagnostics for each inside loop in the history file (Default=4)

DESIGN ..... Controls middle loop diagnostics in the history file (Default=4)

TERM ..... Controls printouts of inside/middle/outside loop iterations in the log file (Default=0)

TXYEST ..... Controls printouts of temperature and composition profile results in input estimate formats in the history file (Default=4)

PLOT

Use to generate stagewise plots of column profiles. Properties can be reported on a MOLE, MASS, or STDVOL basis.

plotno ..... Plot number

plot-list ..... List of non-component-dependent properties to be plotted:

TEMP	Temperature
PRES	Pressure
LRATE	Liquid flow rate. If two liquid phases are present, both are plotted, as is the total liquid flow rate.
VRATE	Vapor flow rate
VL-RATIO	Vapor flow rate/liquid flow rate. If two liquid phases are present, the vapor flow rate/total liquid flow rate is plotted.
LL-RATIO	Second-liquid flow rate/first-liquid flow rate. Available only when two liquid phases are present.

comp-plot ..... Keyword for component-dependent property to be plotted:

X, X1, X2, Y	Fractions of the components and/or component groups listed are plotted. X1 and X2 can be used only when two liquid phases are present.
KVL, KVL1, KVL2, KLL	K-values of the components and/or listed component groups are plotted. KVL1, KVL2, and KLL cause the ratios y/x1, y/x2 and x2/x1 respectively, to be plotted. They can be used only when two liquid phases are present. When two liquid phases are present, KVL is the ratio of vapor component fraction/total liquid component fraction.
REL-VOL	Relative volatilities of the components and/or component groups listed are plotted. You must also specify BASE-COMP. When a component group ID is specified: $$REL-VOL=\frac{\Sigma y_i / \Sigma x_i}{(y/x)_{BASE-COMP}}$$
S-PLOT	Separation factors, defined under S-OPTION

groupid-list ..... List of component IDs and/or component group IDs

BASE-COMP..... Component ID of base component for relative volatility calculations. (Use with the REL-VOL keyword.)

S-OPTION ..... Definition of separation factor:

S-OPTION=LINEAR	Separation factor is defined as: (y_i/x_i) / $(\Sigma y_h/\Sigma x_h)$ if a component ID is specified, or: $(\Sigma y_i/\Sigma x_i)$ / $(\Sigma y_h/\Sigma x_h)$ if a component group ID is specified.
S-OPTION=LOG	Separation factor is defined as: $\ln(x_i/\Sigma x_h)$ if a component ID is specified, or: $\ln(\Sigma x_i/\Sigma x_h)$ if a component group ID is specified. Where: i = Component or list of components specified by a component group; h = Heavy-key component specified by HEAVY-KEY

		S-OPTION=COMBINED	Both linear and log definition are plotted. (Default=LOG)
	HEAVY-KEY		Heavy key component ID or component group ID. (Use with the S-PLOT keyword.)
	BASIS	**BASIS=MOLE**	Plotted values are on a mole basis (Default)
		BASIS=MASS	Plotted values are on a mass basis
		BASIS=STDVOL	Plotted values are on a standard-liquid-volume basis
	ORDER	**ORDER=TOP-DOWN**	Numbers stages from top down (Default)
		ORDER=BOTTOM-UP	Numbers stages from bottom up
	PLOT-HEADING		Heading up to 64 characters enclosed in quotes, printed at the top of the print-plot
	WIDE		Plot width option. Use to override default established by the PLOT-OPTIONS paragraph (See Chapter 46).
SUBROUTINE			Use to specify user-supplied subroutine for KLL. You must also specify NPHASE=3. For details on writing user-supplied subroutines, see *Aspen Plus User Models*, Chapter 16.
	KLL		User-supplied FORTRAN subroutine name for KLL calculations
KLL-USER			Use to specify column segment for which the user-supplied KLL subroutine is used. You must also specify NPHASE=3.
	stage1		Initial stage of a column segment
	stage2		Final stage of a column segment
KLL-VECS			Use to define the length of arrays for the user-supplied KLL subroutine. You must also specify NPHASE=3.
	NINT		Length of integer parameter
	NREAL		Length of real parameter
KLL-INT			Use to enter values for the integer parameter array of the user-supplied KLL subroutine. You must also specify NPHASE=3.
	VALUE-LIST		List of integer values
KLL-REAL			Use to enter values for the real parameter array of the user-supplied KLL subroutine. You must also specify NPHASE=3.
	VALUE-LIST		List of real values
USERK-VECS			Use to define the length of arrays for the user-supplied kinetics subroutine.
	NINT		Length of integer parameter array
	NREAL		Length of real parameter array
	NIWORK		Length of integer workspace array
	NWORK		Length of real workspace array
USERK-INT			Use to enter values for the integer parameter array of the user-supplied kinetics subroutine.
	VALUE-LIST		List of integer values
USERK-REAL			Use to enter values for the real parameter array of the user-supplied kinetics subroutine.
	VALUE-LIST		List of real values

STG-UTL Use to specify optional utilities to provide heating or cooling duty for stage heaters and coolers.

stage..... Stage number.

utilityid ..... Utility ID.

PA-UTL Use to specify optional utilities to provide heating or cooling duty for pumparounds.

pid ..... Pumparound ID.

utilityid ..... Utility ID.

UTILITIES Use to specify optional utilities to provide heating or cooling duty for condenser and reboiler.

COND-UTIL ..... Utility ID for condenser.

REB-UTIL ..... Utility ID for reboiler.

PARAM2 Use to specify salt precipitation handling method.

SALTS Salt precipitation handling option.

SALTS= INCLUDE	Salt reactions defined in the CHEMISTRY will be rigorously handled during column calculations (Default)
SALTS= IGNORE	Salt reactions defined in the CHEMISTRY will not be considered during column calculations.
SALTS= IGNORE-CHECK	Same as the IGNORE option, but the solubility index for the salts on each tray will be checked against the value of SAT-LIMIT and a warning will be issued if the limit is exceeded.

SAT-LIMIT Salt concentration/salt solubility limit (Default=1.0)

Accessing Variables in RADFRAC

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	ID2
PARAM	NSTAGE†	—	—
FEEDS	STAGE	sid	—
PRODUCTS	STAGE, basis–FLOW	sid	—
PSEUDO–STREAM	STAGE, MOLE–FLOW	sid	—
P–SPEC	PRES	stage	—
COL–SPECS	basis–RDV, T1, basis–D, basis–B, D:F, B:F, basis-D:F, basis-B:F, basis–L1, basis-VN, basis–RR, basis-BR, Q1, QN, RW, DP–STAGE, DP–COL, DP-COND, HTLOSS	—	—
PDROP-SEC	PDROP	secno	—
DB:F-PARAMS	STREAMS, COMPS	—	—
SC-REFLUX	DEGSUB, TEMP, OPTION	—	—
THERMOSYPHON	PRES, TEMP, DELT VFRAC, basis-FLOW	—	—
HEATERS	DUTY	stage	—
COOLANT	basis-FLOW, UA, TEMP, PRES	stage	—
HTLOSS-SEC	HTLOSS-SEC	secno	—
HTLOSS	HTLOSS-VAP, HTLOSS-LIQ	—	—
COMP–EFF	EFF	stage	cid
STAGE–EFF	EFF	stage	—
STAGE-EFF-SEC	EFF	secno	—
DECANTERS	L1-SPEC, L2-SPEC, TEMP, DEGSUB	stage	—
L1-RETURN	L1-RFRAC	stage1	stage2
L2-RETURN	L2-RFRAC	stage1	stage2
L1-COMP-EFF	EFF	stage	cid
L2-COMP-EFF	EFF	stage	cid
L1-STAGE-EFF	EFF	stage	—
L2-STAGE-EFF	EFF	stage	—
L2-STAGES	STAGE2	stage1	—
HOLD-UP††	basis-LHLDP, basis-VHLDP	stage1	—
RES-TIME	LTIME, VTIME	stage1	—

† NSTAGE cannot be increased from the value in the Block Paragraph, but it can be decreased.

†† HOLD-UP is in MOLE, MASS or VOL basis.

continued

Block Input (continued)

Sentence	Variables	ID1	ID2
REAC-STAGES	STAGE1, STAGE2, REACID	stage1	
T–EST	TEMP	stage	—
X–EST	X	stage	cid
Y–EST	Y	stage	cid
L–EST	MOLE-FLOW	stage	—
VL–EST	MOLE-RATIO	stage	—
COND–HCURVE	NPOINT, INCR, PDROP	curveno	—
REB–HCURVE	NPOINT, INCR, PDROP	curveno	—
VARY†††	LB, UB, STEP, STAGE, STAGE1, STAGE2, VARY-IC-STRM	varyno	—
SPEC†††	VALUE, SCALE, WEIGHT, STAGE, BASE-STAGE	specno	—
MOLE-KLL	KLL-A, KLL-B, KLL-C, KLL-D	kllno	cid
PUMPAROUND	SOURCE-STAGE, DEST-STAGE, PRES basis-FLOW, TEMP, DELT, DUTY, VFRAC	paid	—

††† Accessed variables are in SI units. VARY-IC-STRM contains pumparound ID.

Block Results

Description	Sentence	Variable	ID1	ID2
Condenser duty	RESULTS	COND–DUTY	—	—
Reboiler duty	RESULTS	REB–DUTY	—	—
Subcooled reflux duty	RESULTS	QSC	—	—
Subcooled temperature	RESULTS	TSC	—	—
Reflux ratio	RESULTS	RR	—	—
Boilup ratio	RESULTS	BR	—	—
Stage temperature	PROFILE	TEMP†	stage	—
Stage pressure	PROFILE	PRES†	stage	—
Stage liquid rate	PROFILE	LRATE†	stage	—
Stage first liquid rate	PROFILE	L1RATE†	stage	—
Stage second liquid rate	PROFILE	L2RATE†	stage	—
Stage vapor rate	PROFILE	VRATE†	stage	—
Stage heat duty	PROFILE	DUTY†	stage	—
Manipulated variables††	MAN–VARS	VALUE†	varyno	—
Liquid compositions	COMPS	X†	cid	stage
First liquid compositions	COMPS	X1†	cid	stage
Second liquid compositions	COMPS	X2†	cid	stage
Vapor compositions	COMPS	Y†	cid	stage
Reaction rates	REAC-RATES	RATE†	stage	cid

† You can also access variables using the VECTOR-DEF sentence. See Chapter 29.

†† Accessed variables are in SI units.

Thermosyphon reboiler:

Description	Sentence	Variable	ID1	ID2
Pressure	REB-RESULTS	PRES	—	—
Temperature	REB-RESULTS	TEMP	—	—
Vapor fraction	REB-RESULTS	VFRAC	—	—
Flow rate	REB-RESULTS	MOLE-FLOW	—	—
Liquid composition	REB-COMP	X†	cid	—
Liquid1 composition	REB-COMP	X1†	cid	—
Liquid2 composition	REB-COMP	X2†	cid	—
Vapor composition	REB-COMP	Y†	cid	—

† You can also access variables using the VECTOR-DEF sentence. See Chapter 29.

Pumparound:

Description	Sentence	Variable†	ID1	ID2
Temperature	PA-RESULTS	TEMP	paid	—
Pressure	PA-RESULTS	PRES	paid	—
Duty	PA-RESULTS	DUTY	paid	—
Vapor fraction	PA-RESULTS	VFRAC	paid	—
Beta	PA-RESULTS	BETA	paid	—
Molar flow rate	PA-RESULTS	MOLE-FLOW	paid	—

† You can also access variables using the VECTOR-DEF sentence. See Chapter 29.

Column Specification Combinations for Two-Phase and Three-Phase Calculations

For rating mode, the column variables that can be specified are variables in the COL-SPECS sentence, and L1-SPEC and L2-SPEC for the first stage in the DECANTERS sentence. The number of variables that can be specified and the allowable combinations of specifications depend on the NPHASE specification in the PARAM sentence.

When NPHASE=2, you must specify either basis-RDV or T1. (T1 is allowed only for columns with a partial condenser, and both a vapor and liquid distillate.) In addition, you must specify two column variables. L1-SPEC and L2-SPEC cannot be used. The allowable combinations of column variables are indicated with an X in Table 15.1:

Table 15.1 Column Specification Combinations for Two-Phase Calculations

	L1	VN	RR	BR	Q1	QN
D	X	X	X	X	X	X
B	X	X	X	X	X	X
D:F	X	X	X	X	X	X
B:F	X	X	X	X	X	X
L1			X	X		
VN			X	X		
RR	X	X		X	X	X
BR	X	X	X		X	X
Q1			X	X		X
QN			X	X	X	

When NPHASE=3, the allowable specifications depend on specifications entered for the top stage decanter. You can choose one of the following specification options:

1 No top stage decanter is present, or only one of L1-SPEC and L2-SPEC is specified for the top stage decanter. You must specify two column variables. The allowable combinations of column variables are indicated with an X in Table 15.2. You must also specify either RDV or T1. T1 is allowed only if the column has no top stage decanter, and there is a partial condenser with both liquid and vapor distillate streams.

2 Both L1-SPEC and L2-SPEC are specified for the top stage decanter. Two column variables must be specified. The allowable combinations are indicated with an X in the previous matrix. Both liquid and vapor distillate are assumed to be present, and RDV is calculated. An initial estimate for RDV is required.

3 Both L1-SPEC and L2-SPEC are specified for the top stage decanter. RDV and one additional column variable must be chosen from the following: D, B, D:F, B:F, Q1, QN.

Option 2 is recommended if free-water calculations are performed and a partial condenser is specified.

Table 15.2 Column Specification Combinations for Three-Phase Calculations

	L1	VN	RR	BR	Q1	QN
D	X	X	X	X	X	X
B	X	X	X	X	X	X
D:F	X	X	X	X	X	X
B:F	X	X	X	X	X	X
Q1						X

MULTIFRAC: Rigorous Fractionation for Complex Columns

Input Language for MULTIFRAC

```
BLOCK  blockid  MULTIFRAC
PROP-SECTIONS  col  stage1  stage2  opsetname  keyword=value
```

Keywords:

FREE-WATER SOLU-WATER HENRY-COMPS CHEMISTRY

```
PARAM  keyword=value
```

Keywords:

NCOL NSTAGE NIC–STREAM

Optional keywords:

ALGORITHM EFF INIT-OPTION HYDRAULIC P-UPDATE P-FIX DAMPING MAXOL TOLOL DSMETH FLASH-MAXIT FLASH-TOL HMODEL2 ILMETH JMETH KBBMAX KMODEL MAXIL MAXIP MAXSBI MAX-BROY PROD-FLASH QMAXBWIL QMAXBWOL QMINBWIL QMINBWOL RMSOL0 RMSOL1 RMSOLJ TOLIL0 TOLILFAC TOLILMIN

```
COL-CONFIG  keyword=value
```

Keywords:

CONDENSER REBOILER KEY-SELECT

```
FEEDS  sid  col  stage  [feed–conv]  / ...
PRODUCTS  sid  col  stage  [PHASE=phase]  [basis–FLOW=value]  / ...
PSEUDO–STREAM  sid  col  stage  [PHASE=phase]  IC–STREAM=ic–stream  &
      [basis–FLOW=value]  / ...
P–SPEC  col  stage  pres  / ...
COL–SPECS  col  keyword=value
```

Keywords:

NSTAGE basis–RDV T1 basis–RR basis–L1 basis–D basis–B Q1 QN RW

Optional keywords:

RDV–EST DP–STAGE DP–COL

```
HEATERS  col  stage  duty
COMP–EFF  col  stage  cid  eff  / ...
STAGE–EFF  col  stage  eff  / ...
```

```
CONNECT–STREAM  ic–stream  SOURCE–COL=source-col  source–stage  &
      DEST–COL=dest-col  dest–stage  keyword=value
```

Optional keywords:

PHASE basis–FLOW TEMP DELT DUTY QSTREAM–IN QSTREAM–OUT

```
L–SPEC  col  stage  keyword=value
```

Keyword:

basis–FLOW

Optional keywords:

Q–COL Q–STAGE IC–STREAM

```
V–SPEC  col  stage  keyword=value
```

Keyword:

basis–FLOW

Optional keywords:

Q–COL Q–STAGE IC–STREAM

```
FLOW–RATIO  rationo  keyword=value
```

Keywords:

basis–RATIO COL STAGE

Optional keywords:

PHASE BASE–COL BASE–STAGE BASE–PHASE Q–COL Q–STAGE IC–STREAM

```
SC–REFLUX  col  keyword=value
```

Keywords:

TEMP DEGSUB

Optional keyword:

OPTION

```
L2-STAGES  col  [stage1]  [stage2] / ...
T–EST  col  stage  temp / ...
L–EST  col  stage  flow / ...
V–EST  col  stage  flow / ...
X–EST  col  stage  cid  x / ...
Y–EST  col  stage  cid  y / ...
REPORT  reportopt-list
```

Special reportopts:

NOPROFILE NOCOMPS NOHYDRAULIC NOENTH TARGET HYDANAL EXTHYD

```
KEY-COMP  col  secno  stage1  stage2  LIGHT-KEY=cid-list  HEAVY-KEY=cid-list
KEY-TOL  col  keyword=value
```

Optional keywords:

KVAL-TOL COMP-TOL SPF-LIMIT STG-SPAN EXCLD-KEY EXG-TREF

TRAY–REPORT *keyword=value*

Optional keywords:

TRAY–OPTION FORMAT ORDER PROPERTIES PRINT–PLOT WIDE

INCL–TRAYS col [stage1] [stage2] / ...
COND–HCURVE curveno col *keyword=value*
REB–HCURVE curveno col *keyword=value*
IC–HTR–HCURVE curveno ic–stream *keyword=value*

Optional keywords:

INDEP–VAR LIST NPOINT INCR HEADING PROPERTIES PRES–PROFILE PDROP PRINT–PLOT HIGH–PRECISION LINES X–SCALE Y–SCALE WIDE GRID INTERPOLATE

VARY varyno vartype [lb] [ub] [step] *keyword=value*

Vartypes:

basis–LPROD basis–VPROD DUTY basis-FEED HEAT–STREAM basis–RDV basis–RR basis–L1 basis–D basis–B Q1 QN RW basis–L basis–V basis–RATIO IC–basis–FLOW IC–TEMP IC–DELT IC–DUTY

Keywords:

COL STAGE STREAM IC–STREAM RATIO–NO

SPEC specno spectype value [scale] [weight] *keyword=value*

Spectypes:

basis–FRAC basis–RECOV basis–FLOW basis–RATIO TEMP DUTY DUTY–RATIO PROP PROP–DIFF PROP–RATIO

Keywords:

COL BASE–COL STAGE BASE–STAGE COMPS BASE–COMPS STREAMS BASE–STREAMS IC–STREAM BASE–IC–STREAM PROPERTY BASE–PROPERTY

Optional keywords:

PHASE BASE–PHASE

DIAGNOSTICS *keyword=value*

Keywords:

MAIN OLVAR1 OLVAR2 CMBAL EMBAL DESIGN TERM TXYEST

PLOT plotno plot–list comp–plot=groupid–list *keyword=value*

Plot-list options:

TEMP PRES LRATE VRATE VL–RATIO

Comp-plot options:

X Y KVL REL–VOL

Optional keywords:

BASE–COMP BASIS ORDER PLOT–HEADING WIDE

IC-UTL *icsid utilityid*
COL-UTL *column stage utilityid*
UTILITIES *column keyword=value / cid keyword=value* **...**

Optional keywords:

COND-UTIL REB-UTIL

Input Language Description for MULTIFRAC

PROP-SECTIONS

Use to specify property options for a column segment. PROP-SECTIONS overrides the PROPERTIES sentence for a column segment. The input language for PROP-SECTIONS is the same as for the PROPERTIES sentence, except that PROP-SECTIONS requires that the column segment be specified. See Chapter 11 for more information about the PROPERTIES sentence.

Column initialization calculations are always performed using the specifications in the PROPERTIES sentence, regardless of the specifications given in the PROP-SECTIONS sentence. Therefore, it is important that the property option in the PROPERTIES sentence gives reasonable property representation at the average condition of the column. Any option set name entered in the PROP-SECTIONS sentence must also be named in the PROPERTIES sentence. (See Chapter 8.)

col..... Column number

stage1..... Initial stage of the column segment

stage2..... Final stage of the column segment

opsetname..... Property option set used for column segment

PARAM

Use to enter the number of columns, total number of stages, number of interconnecting streams, efficiency type, algorithm option, and optional convergence parameters.

NCOL..... Number of columns

NSTAGE..... Total number of stages in all columns, including condensers and reboilers. Must be greater than 1.

NIC-STREAM ..... Number of interconnecting streams. Must be equal to or greater than 1.

ALGORITHM ..... Algorithm convergence options:

ALGORITHM=STANDARD	Standard inside-out formulation, recommended for most applications
ALGORITHM= SUM–RATES	Sum-rates formulation, recommended for wide-boiling systems
ALGORITHM=NEWTON	Newton algorithm, recommended for highly-nonideal systems.

Default is SUM-RATES when INIT-OPTION=CRUDE; otherwise the default is STANDARD.

EFF..... Type of efficiency specified using COMP-EFF or STAGE-EFF keywords:

EFF=VAPOR	Vaporization efficiency (Default)
EFF=MURPHREE	Murphree efficiency

INIT-OPTION ..... Initialization options:

INIT-OPTION=STANDARD	Constant molal overflow, uniform composition profiles (Default)
INIT-OPTION=CRUDE	Applicable to preflash towers, crude towers, FCCU main fractionators, coker fractionators, and vacuum towers

HYDRAULIC Flag to specify whether to perform calculations of hydraulic parameters (for example, flow parameter, reduced vapor throughput, tray loadings, and various transport properties): YES or NO. (Default=NO)

P-UPDATE Update pressure profile during column sizing and rating calculations: YES or NO. (Default=NO)

P-FIX Pressure update option: TOP or BOTTOM. Keeps pressure at column top/bottom constant during pressure updating for column sizing and rating calculations. (Default=TOP)

DAMPING Damping factor. Use to stabilize convergence when excessive oscillation is observed in the convergence behavior:

DAMPING=NONE	No damping (Default)
DAMPING=MILD	Mild level of damping
DAMPING=MEDIUM	Medium level of damping
DAMPING=SEVERE	Severe level of damping. You may need to increase the maximum number of outside loop iterations (keyword MAXOL) to achieve convergence.

MAXOL Maximum number of outside loop iterations (Default=25)

TOLOL Outside loop convergence tolerance (Default=$1x10^{-4}$)

DSMETH Design specification convergence method only for ALGORITHM=STANDARD:

DSMETH=SIMULT	Simultaneous method
DSMETH=NESTED	Nested iteration method (Default)

FLASH-MAXIT Maximum number of feed flash iterations (Default=30)

FLASH-TOL Feed flash tolerance (Default=$1x10^{-4}$)

HMODEL2 Temperature dependence option for local enthalpy departure model. Default selected based on column specifications.

ILMETH Inside loop convergence methods:

ILMETH=BROYDEN	Broyden quasi-Newton method, for ALGORITHM=STANDARD or SUM-RATES (Default for ALGORITHM=STANDARD)
ILMETH=WEGSTEIN	Bounded Wegstein method, for ALGORITHM=STANDARD only
ILMETH=COMBINED	Combination of Broyden and Wegstein methods, for ALGORITHM=STANDARD only
ILMETH=SCHUBERT	Schubert quasi-Newton method, with Powell's dogleg stabilization, for ALGORITHM=SUM-RATES only (Default for ALGORITHM=SUM-RATES)

JMETH Jacobian calculation method for ALGORITHM=SUM-RATES:

JMETH=INIT	Jacobian matrix is computed initially by numerical perturbation. Then the matrix is updated by the Broyden method. (Default)
JMETH=RMSOL	Jacobian matrix is computed by numerical perturbation until outside loop RMS error is below RMSOLJ. Then the matrix is updated by the Broyden method.

KBBMAX Maximum allowable slope value for local average K-value model (Default=-500)

KMODEL ..... Weighting option for local average K-value model:

KMODEL=Y	Vapor mole fraction
KMODEL=X	Liquid mole fraction
KMODEL=K	Vapor mole fraction/(1+K-value) (Default)

MAXIL ..... Maximum number of inside loop iterations per outside loop (Default=10)

MAXIP ..... Maximum number of initialization calculation passes. Default is selected based on the nature of the feed and column specifications.

MAXSBI ..... Maximum number of iterations for component mass balance convergence. Use with ALGORITHM=STANDARD. (Default=10)

MAX-BROY ..... Maximum number of variables converged by the Broyden method in the outside loop. You should not increase MAX-BROY beyond 500. (Default=200)

PROD-FLASH ..... Flash type for product stream in PROP-SET and recycle stream convergence calculations:

PROD-FLASH=PV	Flash with stream pressure and vapor fraction as specifications
PROD-FLASH=TP	Flash with stream temperature and pressure as specifications

(Default is selected based on column specifications.)

QMAXBWIL ..... Maximum value of bounded Wegstein acceleration parameter for inside loop (Default=0.5)

QMAXBWOL ..... Maximum value of bounded Wegstein acceleration parameter for outside loop (Default=0.5)

QMINBWIL ..... Minimum value of bounded Wegstein acceleration parameter for inside loop (Default=0)

QMINBWOL ..... Minimum value of bounded Wegstein acceleration parameter for outside loop (Default=0)

RMSOL0 ..... Threshold value of outside loop RMS error that must be achieved before design specification iterations are performed (Default=0.1)

RMSOL1 ..... Threshold value of outside loop RMS error below which Broyden method is used for selected variables (Default=0.01)

RMSOLJ ..... Value of the outside loop error below which the inside loop Jacobian matrix is updated by the Broyden method. Use with ALGORITHM=SUM-RATES and JMETH=RMSOL. (Default=0.01)

TOLIL0 ..... Initial value of inside loop tolerance (Default=0.01)

TOLILFAC ..... Ratio of inside loop tolerance to outside loop RMS error (Default=0.05)

TOLILMIN ..... Minimum value of inside loop tolerance (Default=$1x10^{-6}$)

COL-CONFIG

Use to enter column configuration choices. These include condenser and reboiler configurations and the method for selecting key-components for column targeting analysis. If you specify the condenser configuration, you do not need to specify distillate vapor fraction (RDV) in the COL-SPECS sentence, except for partial condensers with both vapor and liquid distillates. You can choose any of the four condenser types for the first column. For all other columns, only two types (NONE and PARTIAL-V) are available.

CONDENSER ..... Condenser configuration

CONDENSER=TOTAL	Total condenser with a liquid distillate (RDV=0)

	CONDENSER=PARTIAL-V	Partial condenser with vapor distillate only (RDV=1)
	CONDENSER= PARTIAL-V-L	Partial condenser with vapor and liquid distillates (0<RDV<1)
	CONDENSER=NONE	No condenser. Reflux is provided by an external feed or pumparound return to the top stage (condenser heat duty=0; RDV=1)

REBOILER ..... Reboiler configuration

REBOILER=KETTLE	Kettle type reboiler (Default)
REBOILER=NONE	No reboiler (reboiler heat duty=0). Boilup is provided by external feed or pumparound return to the bottom stage.

KEY-SELECT ..... Method for selection of light and heavy key components for column targeting analysis. Specify KEY-SELECT if TARGET or HYDANAL report option is selected in the REPORT sentence.

KEY-SELECT=USER	Use light and heavy key components specified in KEY-COMP sentence.
KEY-SELECT= SPLIT-FRACTION	Select the light and heavy key components on the basis of component split-fractions in column product streams. This method is best suited for sharp or near-sharp splits.
KEY-SELECT=K-VALUE	Select the light and heavy key components on the basis of component K-values. This method is best suited for sloppy splits. (Default)
KEY-SELECT= COMP-PROFILE	Select the light and heavy key components on the basis of composition profiles. In principle, this method is similar to KEY-SELECT= K-VALUE. It is best suited for sloppy splits and it is, in general, inferior to KEY-SELECT= K-VALUE.

FEEDS

Use to enter inlet material and heat stream locations, and feed conventions for material streams.

sid..... Stream ID

col..... Column number

stage..... Stage number

feed–conv	**ABOVE–STAGE**	Introduces feed between stages, above designated stage (Default)
	ON–STAGE	Introduces feed on designated stage

PRODUCTS

Use to enter stream locations for material and heat outlet streams.

For a material stream, you can enter the phase specification. The phase specification for the distillate of column 1 must be consistent with the specified value of RDV. When RDV does not equal zero or unity, or is a manipulated variable, or when T1 is specified in COL-SPECS, two distillate streams are required: one vapor and one liquid. You can specify a separate product stream for the free-water distillate from column 1. If you do not specify a separate stream, the free-water distillate is mixed with the organic liquid distillate phase.

The flow rates of vapor and liquid distillates for column 1, vapor distillate for other columns, and bottoms of all columns are not specified in the PRODUCTS statement. They are either calculated or specified in a COL-SPECS, L-SPEC or V-SPEC statement. When L2-STAGES is not specified, *phase*=W is allowed for *stage1* only. The amount of decant water is determined by RW. When L2-STAGES is specified, *phase*=W is allowed for any stage included in L2-STAGES, and corresponds to the entire free-water phase in the specified stages.

sid..... Stream ID

col..... Column number

stage..... Stage number

PHASE..... **PHASE=L** Liquid (Default)

PHASE=V Vapor

PHASE=W Free-water

PHASE=L1 Organic phase

PHASE=TL Total drawoff of stage liquid

PHASE=TV Total drawoff of stage vapor

basis-FLOW..... Flow rate on MOLE, MASS, or STDVOL basis. Not allowed for *phase*=W. When *phase* is TL and TV, specified value is treated as initial estimate only.

PSEUDO-STREAM

Use to identify an outlet stream as a pseudoproduct stream, and to specify the internal stream or interconnecting stream whose compositions and conditions are to be represented by the pseudostream. You must enter either *col* and *stage*, or IC-STREAM.

sid..... Stream ID

col..... Column number

stage..... Stage number

PHASE..... **PHASE=L** Liquid (Default)

PHASE=V Vapor

PHASE=W Free-water

PHASE=L1 Organic phase

PHASE=TL Total liquid

PHASE=TV Total vapor

IC-STREAM ..... Interconnecting stream number. You cannot use IC-STREAM, if you specified *col*, *stage*, or *phase*.

basis-FLOW..... Flow rate of pseudoproduct stream on MOLE, MASS, or STDVOL basis. If you did not supply a value, the net flow of the internal stream (excluding any sidedraw) or the interconnecting stream flow rate is used.

P-SPEC

Use to enter the column pressure profile. Enter one P-SPEC statement for each column.

col..... Column number

stage..... Stage number

pres ..... Pressure

COL-SPECS

Use to enter the number of stages and additional specifications for each column. Tables 15.3 and 15.4 list the valid column specification combinations. For column 1, COL-SPECS is used to specify the distillate vapor fraction (RDV), or the top stage temperature (T1), and an initial estimate of RDV. If free-water calculations are performed, the free-water reflux ratio (RW) is also specified.

You can also enter the column pressure drop or pressure drop per stage. For design mode, any of the quantities specified in a COL-SPECS statement (with the exception of NSTAGE, T1, RDV-EST, DP-STAGE, and DP-COL) can be treated as manipulated variables, in which case the values given in the COL-SPECS statement are initial guesses. An input heat stream to the top or bottom stage of a column can be used in place of Q1 or QN, respectively. Substitute MOLE, MASS, or STDVOL for the word *basis* in the following specifications.

col..... Column number

NSTAGE..... Number of stages. Must be greater than 1 for column 1.

basis-RDV ..... Distillate vapor fraction. RDV=DV/D where DV is the distillate vapor flow rate and D is the total distillate flow rate (excluding free-water). (Use for column 1 only.)

T1 ..... Temperature of top stage. (Use for column 1 only.)

basis-RR ..... Reflux ratio (excluding free-water) (L1/D, where L1 is the reflux rate excluding free-water)

basis-L1 ..... Top stage liquid flow rate including the liquid distillate (excluding free-water)

basis-D ..... Distillate flow rate (excluding free-water). For column 1, D includes both vapor and liquid distillate flows. For other columns, D includes vapor distillate only. Liquid distillate flow, if present, is specified in the PRODUCTS sentence.

basis-B..... Bottoms flow rate

Q1..... Condenser (or top stage) heat duty

QN ..... Reboiler (or bottom stage) heat duty

RW..... Free-water reflux ratio. RW=LW'/DW, where LW' is the free-water reflux rate and DW is the free-water distillate rate. (Default=0)

RDV-EST ..... Estimate of the molar distillate vapor fraction. (Use for column 1 only.)

DP-STAGE ..... Pressure drop per stage

DP-COL ..... Pressure drop for column

HEATERS

Use to enter the heater stage locations and duties. You can use input heat streams instead of a heater.

col..... Column number

stage..... Stage number

duty ..... Heat duty

COMP-EFF

Use to enter component efficiency. You cannot use COMP-EFF if you specified STAGE-EFF. The type of efficiency is specified by EFF in the PARAM statement.

col..... Column number

stage..... Stage number

cid..... Component ID

eff..... Efficiency (Default=1)

STAGE-EFF

Use to enter stage efficiency. These efficiencies are applied to all components on the stage. You cannot use STAGE-EFF if you specified COMP-EFF. The type of efficiency is specified by EFF in the PARAM statement.

col..... Column number

stage..... Stage number

eff..... Efficiency (Default=1)

CONNECT-STREAM

Use to enter the source, destination, phase, flow rate, and thermal condition of each interconnecting stream. There can be any number of interconnecting streams from the same source column, stage, and phase, and any number with the same destination column and stage. Interconnecting streams are introduced on the destination stage regardless of their phase (feed-conv=ON-STAGE). Enter one CONNECT-STREAM statement for each interconnecting stream.

The vapor leaving the top stage of a column and the liquid leaving the bottom stage are referred to as terminal streams. Each terminal stream can be the source of a product stream and any number of interconnecting streams. If there is no product stream, at least one interconnecting stream must have an unspecified flow. Any of the interconnecting streams can have a heater with heat duty, temperature or temperature change specified.

An internal stream can be the source of any number of interconnecting streams, any of which can have a heater. If an interconnecting stream does not have an external heater, the flow rate must be specified directly in the CONNECT-STREAM sentence, or fixed indirectly by an L-SPEC, V-SPEC or FLOW-RATIO sentence.

If an interconnecting stream has a heater, two of the following variables must be specified: flow rate, temperature (or temperature change), and heat duty. If you specified heat duty and temperature (or temperature change), the flow rate is calculated. Temperature change cannot be zero. Note that if the flow rate is fixed indirectly by an L-SPEC, V-SPEC, or FLOW-RATIO sentence, only one variable among duty, temperature, or temperature change can be given.

ic-stream	Interconnecting stream number; must be sequential starting with 1.	
source-col	Source column number	
source-stage	Source stage number	
dest-col	Destination column number	
dest-stage	Destination stage number	
PHASE	**PHASE=L**	Liquid (Default)
	PHASE=V	Vapor
basis-FLOW	Flow rate on MOLE, MASS, or STDVOL basis	
TEMP	Temperature	
DELT	Change in temperature	
DUTY	Heat duty	
QSTREAM-IN	Inlet heat stream ID	
QSTREAM-OUT	Outlet heat stream ID	

L-SPEC, V-SPEC

Use to specify liquid and vapor flows, of terminal streams or internal streams. A specified value can be zero to model a total drawoff if there is a product or interconnecting stream of the same phase leaving the stage.

The heat duty associated with the heater of the same stage or another stage (using Q-COL and Q-STAGE) or the flow rate of an associated interconnecting stream (specified by IC-STREAM) must be allowed to vary so that enthalpy and mass balances can be satisfied. An initial guess for the associated heat duty or interconnecting stream flow rate is not needed. The calculated heat duty can be placed in an outlet heat stream using a PRODUCTS sentence.

For a terminal stream: L-SPEC and V-SPEC refer to the net flow of the stream excluding any portions withdrawn by interconnecting streams with flow specifications. Flow specifications include direct specifications and those that are fixed indirectly by the associated heater specifications or other L-SPEC or V-SPEC statements.

For an internal stream: L-SPEC and V-SPEC refer to the net flow of the stream excluding any portions withdrawn as products or interconnecting streams.

col..... Column number

stage..... Stage number for specified flow

basis-FLOW..... Flow rate on MOLE, MASS, or STDVOL basis

Q-COL ..... Column number for the associated heater (Default=*col*)

Q-STAGE ..... Stage number for the associated heater (Default=*stage*)

IC-STREAM ..... Interconnecting stream number for the associated interconnecting stream

FLOW-RATIO

Use to specify the ratio of two flow rates, $FLOW_I/FLOW_J$. The flows can be of different phases and come from any stage of any column. The flows refer to the net flow from a stage and follow the same convention as that described for L-SPEC and V-SPEC in handling internal and terminal streams.

When you specify a flow ratio, the heat duty associated with the heater of the same stage or another stage (using Q-COL and Q-STAGE), or the flow rate of an associated interconnecting stream (specified by IC-STREAM), must be allowed to vary so that enthalpy and mass balances can be satisfied. You can place the calculated heat duty in an outlet heat stream using a PRODUCTS sentence.

rationo..... Flow ratio number

basis-RATIO..... Flow ratio on a MOLE, MASS or STDVOL basis

COL..... Column number for $FLOW_I$

STAGE..... Stage number for $FLOW_I$

PHASE..... Phase code for $FLOW_I$:

PHASE=L	Liquid (Default)
PHASE=V	Vapor

BASE-COL ..... Column number for $FLOW_J$ (Default=COL)

BASE-STAGE ..... Stage number for $FLOW_J$ (Default=STAGE+1)

BASE-PHASE ..... Phase code for $FLOW_J$:

BASE-PHASE=L	Liquid
BASE-PHASE=V	Vapor (Default)

Q-COL ..... Column number for associated heater (Default=COL)

Q-STAGE ..... Stage number for associated heater (Default=STAGE+1)

IC-STREAM ..... Interconnecting stream number for the associated interconnecting stream

SC-REFLUX

Use to specify either the degrees subcooling of the reflux or the reflux temperature. If you do not give an SC-REFLUX statement, the reflux is assumed to be a saturated liquid. SC-REFLUX is allowed only for column 1.

col..... Column number; must be column 1

TEMP..... Reflux temperature

DEGSUB ..... Degrees subcooling

OPTION..... **OPTION=0** Both reflux and liquid distillate are subcooled (Default)

OPTION=1 Only reflux is subcooled

L2-STAGES

Use to indicate a segment of stages to be tested for free-water calculations. You must specify FREE-WATER=YES globally using the SIM-OPTIONS paragraph (see Chapter 45), or locally for the MULTIFRAC block, using the BLOCK-OPTIONS sentence (see Chapter 11).

col..... Column number

stage1..... Initial stage of a column segment for which free-water calculations are performed

stage2..... Final stage of a column segment for which free-water calculations are performed

T-EST

Use to enter an initial temperature profile for each column. For INIT-OPTION=STANDARD, top stage and bottom stage estimates are required. For INIT-OPTION=CRUDE, if bottoms flow rates of all columns are either specified or estimated, no temperature estimate is required. It is recommended, however, that you provide temperature estimates if available.

col..... Column number

stage..... Stage number

temp ..... Temperature

L-EST, V-EST

Use to enter initial estimates of liquid and vapor mole flow profiles. The flow entered is the total flow of the respective phase, including any portions withdrawn as products or interconnecting streams. L-EST and V-EST are generally not needed. If you specified Q1 and QN for a column, you should provide an estimate of the liquid flow for the bottom stage unless you specified the liquid flow in the COL-SPECS or L-SPEC sentence.

col..... Column number

stage..... Stage number

flow ..... Molar flow rate

X-EST, Y-EST

Use to enter initial estimates of column composition profiles. If you entered X-EST and Y-EST for any column, you must enter them for all columns. X-EST and Y-EST are generally not required, but can be used as a convergence aid. X-EST and Y-EST are always used together.

col..... Column number

stage..... Stage number

cid..... Component ID

x ..... Liquid mole fraction

y ..... Vapor mole fraction

REPORT Use to override the default report options. You can use the standard REPORT options for use within a block (see Chapter 11) for MULTIFRAC.

reportopt ..... Standard block report options (see Chapter 11), in addition to the following:

NOPROFILE	Suppress the stagewise profiles of temperature, operating pressure, flows, enthalpies, and duties for this block
NOCOMPS	Suppress the mole fraction and K-value profiles for this block
NOHYDRAULIC	Suppress the hydraulic parameters reported for this block
NOENTH	Suppress the enthalpy profile for this block
TARGET	Include column targeting thermal analysis results
HYDANAL	Include column targeting hydraulic analysis results
EXTHYD	Include extended hydraulic parameter report. Use only when NOHYDRAULIC report option is not selected or when HYDRAULIC=YES in the PARAM sentence.

KEY-COMP Use to specify light and heavy key components for column targeting analysis. Use only when TARGET and/or HYDANAL report option is selected and KEY-SELECT=USER in the COL-CONFIG sentence for the column under consideration.

col..... Column number

secno ..... Section number for key component specification

stage1..... Stage number for the initial stage of the section

stage2..... Stage number for the final stage of the section

LIGHT-KEY ..... List of light key components

HEAVY-KEY ..... List of heavy key components

KEY-TOL Use to specify tolerances and other parameters for light and heavy key component selection methods other than KEY-SELECT=USER and for exergy loss calculations. Use only when TARGET and/or HYDANAL report option is selected.

col..... Column number

KVAL-TOL..... Tolerance on component K-values. Specify when KEY-SELECT= K-VALUE or SPLIT-FRACTION. (Default=$1x10^{-5}$)

COMP-TOL..... Tolerance on component mole-fractions. Specify when KEY-SELECT=
K-VALUE, SPLIT-FRACTION, or COMP-PROFILE. (Default=$1x10^{-6}$)

SPF-LIMIT..... Minimum value of component split-fractions, in the top and the bottom products of a column section, necessary for key component selection. Specify when KEY-SELECT=SPLIT-FRACTION. (Default=0.9)

STG-SPAN ..... Stage span for computing composition profiles. Specify when KEY-SELECT=COMP-PROFILE. (Default=2)

EXCLD-KEY..... List of components to be excluded from key component selection. Specify when KEY-SELECT=K-VALUE, SPLIT-FRACTION, or COMP-PROFILE.

EXG-TREF..... Reference temperature for exergy loss calculations (Default=298.15 K)

TRAY-REPORT

Use to specify the format of the report and additional tray properties to be reported (in addition to the flows, temperatures, pressures, enthalpies, duties, mole fractions, and K-values printed in the standard report).

TRAY-OPTION	Specifies stages included in the report:	
	TRAY-OPTION=BRIEF	Reports the stages that have feeds, products, heaters, pumparounds, bypasses, interconnecting streams, and maximum and minimum flows, and the stages immediately above and below those stages (Default)
	TRAY-OPTION= INCL–TRAYS	Reports the stages specified in the INCL-TRAYS statement
	TRAY-OPTION= ALL–TRAYS	Reports all trays
FORMAT	**FORMAT=PROFILE**	Prints tabular column profiles (Default)
	FORMAT=STAGE	Prints individual stage reports
	FORMAT=COMBINED	Prints both tabular column profiles and individual stage reports
ORDER	Tray numbering order. Use for report only.	
	ORDER=TOP-DOWN	Numbers stages from top down (Default)
	ORDER=BOTTOM-UP	Numbers stages from bottom up
PROPERTIES	List of property set IDs	
WIDE	Report width option	
	WIDE=YES	Produces wide (132 columns) reports (Default)
	WIDE=NO	Produces standard (80 columns) reports

INCL-TRAYS

Use to designate trays to be included in the report when TRAY-OPTION=INCL-TRAYS. One INCL-TRAYS statement is entered for each column for which tray reports are desired. If you enter a column number without stage numbers, all stages are reported for that column.

col.....	Column number
stage1.....	Initial stage of column segment to be reported
stage2.....	Final stage of column segment to be reported (Default=*stage1*)

COND-HCURVE, REB-HCURVE

Use to generate cooling/heating curve tables for the condenser or reboiler of any column. If you specify efficiency for a condenser (or reboiler) using COMP-EFF or STAGE-EFF, cooling (or heating) curves calculated for that condenser (or reboiler) will not be consistent with column results. You must specify the column number. See Chapter 11 for a description of input keywords.

col.....	Column number

IC-HTR-HCURVE

Use to generate heating or cooling curve tables for the external heater associated with any interconnecting stream, pumparound, or bypass. If you specify efficiency for the source stage of an interconnecting stream using COMP-EFF or STAGE-EFF, heating and cooling curves calculated for that interconnecting stream will not be consistent with column results. You must specify the interconnecting stream number. See Chapter 11 for a description of input keywords.

ic–stream.....	Interconnecting stream number

VARY

Use to specify manipulated variables for the design mode. You must provide initial guesses of the manipulated variables. basis-FEED and HEAT–STREAM are initialized in a STREAM paragraph. For all other manipulated variables, enter estimates using the usual rating mode specification keywords:

Sentence	Variables
PRODUCTS	LPROD and VPROD
HEATERS	DUTY
CONNECT-STREAM	IC-FLOW, IC-TEMP, IC-DELT, and IC-DUTY
L-SPEC	L
V-SPEC	V
FLOW-RATIO	RATIO
COL-SPECS	All others

For DSMETH=NESTED, you must supply lower and upper bounds (*lb* and *ub*) and initial guesses must be bracketed by the bounds. Enter one VARY statement for each manipulated variable. Substitute MOLE, MASS, or STDVOL for the word *basis*.

varyno ..... Manipulated variable number

vartype ..... Manipulated variable type:

basis-LPROD	Liquid sidestream product flow rate of a column (specified by COL) and a stage (specified by STAGE)
basis-VPROD	Vapor sidestream product flow rate of a column (specified by COL) and a stage (specified by STAGE)
DUTY	External heater duty of a column (specified by COL) and a stage (specified by STAGE)
basis-FEED	Feed flow rate in MOLE, MASS, or STDVOL basis (specified by STREAM)
HEAT-STREAM	Duty of a feed heat stream (specified by STREAM)
basis-RDV	Distillate vapor fraction (RDV=DV/D, where DV is the distillate vapor flow rate and D is the total distillate flow rate, excluding any free-water)
basis-RR	Reflux ratio, excluding free-water (L1'/D)
basis-L1	Top stage liquid flow rate (excluding free-water)
basis-D	Distillate flow rate (excluding free-water). For column 1, D includes both vapor and liquid distillate flows. For other columns, D includes vapor distillate only. Liquid distillate flow (if present) is specified in the PRODUCTS statement.
basis-B	Bottoms flow rate
Q1	Condenser (or top stage) heat duty
QN	Reboiler (or bottom stage) heat duty
RW	Free-water reflux ratio. RW=LW'/DW, where LW' is the free-water reflux rate and DW is the free-water distillate rate
basis-L	Liquid flow rate of a column (specified by COL) and a stage (specified by STAGE)
basis-V	Vapor flow rate of a column (specified by COL) and a stage (specified by STAGE)
basis-RATIO	Ratio of 2 flows defined by a FLOW-RATIO sentence (specified by RATIO-NO)

IC-basis-FLOW Flow rate of an interconnecting stream (specified by IC-STREAM)

IC-TEMP Temperature of an interconnecting stream (specified by IC-STREAM)

IC-DELT Temperature change of an interconnecting stream (specified by IC-STREAM)

IC-DUTY Heat duty of an interconnecting stream (specified by IC-STREAM)

lb ..... Lower bound. Use for DSMETH=NESTED only.

ub ..... Upper bound. Use for DSMETH=NESTED only.

step ..... Maximum step size. Use for DSMETH=NESTED only. (Default=0.1*(ub–lb))

COL ..... Column number (required for all *vartypes*) except HEAT-STREAM, basis-RATIO, basis-IC-FLOW, IC-TEMP, IC-DELT, and DUTY.

STAGE ..... Stage number (required for *vartypes* LPROD, VPROD, L, V, and DUTY)

STREAM ..... Stream ID (required for *vartypes* basis-FEED and HEAT-STREAM)

IC-STREAM ..... Interconnecting stream number (required for *vartypes* IC-basis-FLOW, IC-TEMP, IC-DELT and IC-DUTY)

RATIO-NO ..... Flow ratio number (required for *vartype* RATIO)

SPEC

Use to enter design specifications. Enter one SPEC sentence for each design specification. For DSMETH=NESTED, the number of SPEC sentences must be greater than or equal to the number of VARY sentences. For DSMETH=SIMULT, the number of SPEC sentences must be equal to the number of VARY sentences. Substitute MOLE, MASS, or STDVOL for the word *basis*.

specno ..... Design specification number

spectype ..... Design specification type:

basis-FRAC Purity of a product stream (specified by STREAMS) or an internal stream (specified by COL, STAGE, and PHASE)
FRAC = $\Sigma x_i / \Sigma x_j$
Where:
x = Component fraction
i = Component in the COMPS list
j = Component in the BASE–COMPS list
The default for BASE–COMPS is all components (Σx_j=1).

basis-RECOV Component recovery. RECOV = $\Sigma\Sigma f_{ij} / \Sigma\Sigma f_{ik}$
Where:
f = Component flow rate
i = Component in the COMPS list
j = Product stream in the STREAMS list
k = Feed stream in the BASE-STREAMS list.
The default for BASE-STREAMS is all feed streams.

basis-FLOW Flow rate of a group of components (specified by COMPS) in a set of product streams (specified by STREAMS) or an internal stream (specified by COL, STAGE, and PHASE). The default for COMPS is all components.

	basis-RATIO	RATIO=$\Sigma f_{i1}/\Sigma f_{j2}$ (BASE-STAGE specified) or $\Sigma f_{i1}/\Sigma f_{jk}$ (BASE-STREAMS specified or defaulted)

For basis-RATIO:

i = Component in the COMPS list

j = Component in the BASE-COMPS list

k = Stream in the BASE-STREAMS list

f_{i1} = Component *i* flow rate in an internal stream specified by COL, STAGE and PHASE

f_{j2} = Component *j* flow rate in an internal stream specified by BASE-COL, BASE-STAGE and BASE-PHASE

f_{jk} = Component *j* flow rate in a feed or product stream in the BASE-STREAMS list. (The BASE-STREAMS list cannot mix feed and product streams.)

The default for COMPS and BASE-COMPS is all components, and the default for BASE-STREAMS is all feed streams.

TEMP	Temperature on a given STAGE of a given COL
DUTY	Heat duty of a stage (specified by COL and STAGE) or interconnecting stream (specified by IC–STREAM)
DUTY-RATIO	*Q1* divided by *Q2* Where: *Q1* = Heat duty of a stage (specified by COL and STAGE) or interconnecting stream (specified by IC-STREAM). *Q2* = Heat duty of a stage (specified by BASE-COL and BASE-STAGE) or interconnecting stream (specified by BASE-IC-STREAM)
PROP	Property value, as specified by PROPERTY, for a product stream (specified by STREAMS) or an internal stream (specified by COL, STAGE, and the property phase qualifier in the corresponding PROP-SET paragraph)
PROP-DIFF	Property value minus base property value, as specified by PROPERTY and BASE-PROPERTY. PROPERTY is the property of a product stream (specified by STREAMS) or of an internal stream (specified by COL, STAGE, and the phase qualifier in the corresponding PROP-SET paragraph). BASE-PROPERTY is the property of a product stream (specified by BASE-STREAMS) or of an internal stream (specified by BASE-COL, BASE-STAGE, and the phase qualifier in the corresponding PROP-SET paragraph).
PROP–RATIO	Ratio of property value to base property value, as specified by PROPERTY and BASE-PROPERTY. PROPERTY and BASE-PROPERTY are as defined for PROP-DIFF.

value..... Desired value of the design specification

scale..... Scale factor (Default=1)

weight..... Weighting factor. Use for DSMETH=NESTED only. (Default=1)

COL..... Column number

BASE-COL..... Column number

STAGE..... Stage number

BASE-STAGE ..... Stage number

COMPS ..... List of component IDs

BASE-COMPS..... List of component IDs

STREAMS ..... List of stream IDs

BASE-STREAMS..... List of stream IDs

IC-STREAM ..... Interconnecting stream number

BASE-IC-STREAM..... Interconnecting stream number

PROPERTY ..... ID of a property set defined by a PROP-SET paragraph consisting of a single scalar property. (See Chapter 41.)

BASE-PROPERTY..... ID of a property set defined by a PROP-SET paragraph consisting of a single scalar property. (See Chapter 41.)

PHASE.....	**PHASE=L**	Liquid (Default)
	PHASE=V	Vapor
	PHASE=W	Free water
BASE-PHASE	**BASE-PHASE=L**	Liquid
	BASE-PHASE=V	Vapor (Default)
	BASE-PHASE=W	Free water

DIAGNOSTICS Use to control the level of convergence diagnostics printed in the history and log files. You can enter a level between 0 and 10. The amount of diagnostics increases with each level.

MAIN ..... Controls printouts of initial/final profiles, inside/middle/outside loop iterations, and outside loop variables/functions in the history file (Default=4)

OLVAR1..... Controls initial local model parameter diagnostics in the history file (Default=4)

OLVAR2..... Controls local model parameter diagnostics for each outside loop in the history file (Default=4)

CMBAL ..... Controls component mass balance diagnostics for each inside loop in the history file (Default=4)

EMBAL..... Controls enthalpy balance diagnostics for each inside loop in the history file (Default=4)

DESIGN..... Controls middle loop diagnostics in the history file (Default=4)

TERM ..... Controls printouts of inside/middle/outside loop iterations in the log file (Default=0)

TXYEST ..... Controls printing of temperature and composition profile results in input estimate formats in the history file (Default=4)

PLOT Use to generate stagewise plots of column profiles. Properties can be reported on a MOLE, MASS, or STDVOL basis.

plotno ..... Plot number

plot-list..... List of non-component-dependent properties to be plotted:

TEMP	Temperature
PRES	Pressure
LRATE	Liquid flow rate
VRATE	Vapor flow rate
VL-RATIO	Vapor flow rate/liquid flow rate

comp-plot ..... Keyword for component-dependent property to be plotted:

X, Y	Fractions of the components and/or component groups listed are plotted.
KVL	K-values of the components and/or component groups listed are plotted.
REL–VOL	Relative volatilities of the components and/or component groups listed are plotted. You must also specify BASE-COMP. When a component group ID is specified, $$REL-VOL = \frac{\Sigma y_i / \Sigma x_i}{(y/x)_{BASE-COMP}}$$

groupid-list ..... List of component IDs and/or component group IDs

BASE-COMP..... Component ID of base component for relative volatility calculations. (Use with the REL-VOL keyword.)

BASIS	**BASIS=MOLE**	Plotted results are on a mole basis (Default)
	BASIS=MASS	Plotted results are on a mass basis
	BASIS=STDVOL	Plotted results are on a standard-liquid-volume basis
ORDER	**ORDER=TOP-DOWN**	Numbers stages from top down (Default)
	ORDER=BOTTOM-UP	Numbers stages from bottom up

PLOT-HEADING..... Heading up to 64 characters included in quotes, printed at the top of the print-plot

WIDE ..... Plot width option. Use to override default established by the PLOT-OPTIONS paragraph (See Chapter 46).

IC-UTL

Use to specify optional utilities to provide heating or cooling duty for interconnecting streams.

icsid ..... Interconnecting stream ID.

utilityid ..... Utility ID.

COL-UTL

Use to specify optional utilities to provide heating or cooling duty for stage heaters and coolers.

column..... Column ID.

stage..... Stage number.

utilityid ..... Utility ID.

UTILITIES

Use to specify optional utilities to provide heating or cooling duty for condensers and reboilers.

column..... Column ID.

COND-UTIL ..... Utility ID for condenser.

REB-UTIL ..... Utility ID for reboiler.

Accessing Variables in MULTIFRAC

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	ID2	ID3
PARAM	NSTAGE	—	—	—
FEEDS	COL, STAGE	sid	—	—
PRODUCTS	COL, STAGE, basis–FLOW	sid	—	—
PSEUDO–STREAM	COL, STAGE, IC–STREAM, basis–FLOW	sid	—	—
P–SPEC	PRES	col	stage	—
COL–SPECS	NSTAGE, basis–RDV, T1, basis–RR, basis–L1, basis–D, basis–B, Q1, QN, RW, RDV–EST, DP–STAGE, DP–COL	col	—	—
HEATERS	DUTY	col	stage	—
COMP–EFF	EFF	col	stage	cid
STAGE–EFF	EFF	col	stage	—
CONNECT–STREAM	SOURCE–COL, SOURCE–STAGE, DEST–COL, DEST–STAGE, basis–FLOW, TEMP, DELT, DUTY	ic–stream	—	—
L–SPEC	basis–FLOW, Q–COL, Q–STAGE, IC–STREAM	col	stage	—
V–SPEC	basis–FLOW, Q–COL, Q–STAGE, IC–STREAM	col	stage	—
FLOW–RATIO	basis–RATIO, COL, STAGE, BASE–COL, BASE–STAGE, Q–COL, Q–STAGE, IC–STREAM	rationo	—	—
SC–REFLUX	TEMP, DEGSUB	col	—	—
T–EST	TEMP	col	stage	—
L–EST	FLOW	col	stage	—
V–EST	FLOW	col	stage	—
X–EST	X	col	stage	cid
Y–EST	Y	col	stage	cid
COND–HCURVE	NPOINT, INCR, PDROP	curveno	—	—
REB–HCURVE	NPOINT, INCR, PDROP	curveno	—	—
IC–HTR–HCURVE	NPOINT, INCR, PDROP	curveno	—	—
VARY†	LB, UB, STEP, COL, STAGE, IC–STREAM, RATIO-NO	varyno	—	—
SPEC†	VALUE, SCALE, WEIGHT, COL, STAGE, IC–STREAM	specno	—	—

† Accessed variables are in SI units.

Block Results

Description	Sentence	Variable†	ID1	ID2
Reflux ratio	RESULTS	RR	col	—
Boilup ratio	RESULTS	BR	col	—
Condenser duty	RESULTS	COND–DUTY	col	—
Reboiler duty	RESULTS	REB–DUTY	col	—
Stage temperature	PROFILE	TEMP	stack stage††	—
Stage liquid flow	PROFILE	LRATE	stack stage††	—
Stage vapor flow	PROFILE	VRATE	stack stage††	—
Stage heat duty	Q-PROFILE	QCAL	stack stage††	—
Manipulated variable†††	MAN–VARS	VALUE	—	—
Liquid compositions	COMPS	X	stack stage††	cid
Liquid1 compositions	COMPS	X1	stack stage††	cid
Vapor compositions	COMPS	Y	stack stage††	cid

† You can also access variables using the VECTOR-DEF sentence. See Chapter 29.

†† Stack stage is the stage number if all columns are stacked one on top of another to form one column. For example, if there are 2 columns and both columns have 10 stages, stage 5 in column 2 has a stack stage number of 15.

††† Accessed variables are in SI units.

Column Specification Combinations for Column 1 and Other Columns

The allowable combinations of column variables are different for column 1 and the other columns.

Allowable combinations are indicated with an X in the following matrices:

Table 15.3 Column Specification Combinations for Column 1

	L1	RR	Q1	QN
D	X	X	X	X
B	X	X	X	X
Q1				X

Table 15.4 Column Specification Combinations for Other Columns

	L1	Q1	QN
D	X	X	X
B	X	X	X
Q1			X

For special cases where the column has only one stage, you must specify only one of the following variables: D, B, or Q1.

PETROFRAC: Petroleum Refining Fractionation

Input Language for PETROFRAC

```
BLOCK    blkid    PETROFRAC
SUBOBJECTS    keyword=value
```

Keywords:

PUMPAROUND STRIPPER

```
PROP-SECTIONS    stage1    stage2    opsetname    keyword=value
```

Keywords:

FREE-WATER SOLU-WATER HENRY-COMPS

```
PARAM    keyword=value
```

Keywords:

NSTAGE NPA NSTRIP NSSTRIP

Optional keywords:

EFF HYDRAULIC P-UPDATE P-FIX DAMPING MAXIT TOL METHOD ALGORITHM THERM-EFF INIT-OPTION DSMETH FLASH-MAXIT FLASH-TOL FLOW-RF2 HMODEL2 INCL-THEFF KBBMAX KMODEL MAX-BROY MAXIL MAXIO MAXIP NHOMOTOPY PROD-FLASH QMAXBWIL QMAXBWOL QMINBWIL QMINBWOL RMSOL0 RMSOL1 STOR-FACTOR TOLIL0 TOLILFAC TOLILMIN JMETH RMSOLJ TOLILO

```
COL-SPECS    keyword=value
```

Keywords:

CONDENSER REBOILER T1 basis-RR basis-L1 basis-D basis-B Q-COND Q-REB DEGSUB KEY-SELECT

Optional keywords:

DP-STAGE DP-COL basis-DV:D STEAM STEAM:PROD

```
FEEDS    sid    stage    [feed-conv]  /  . . .
PRODUCTS    sid    stage    [phase]    [basis-FLOW=value]  /  . . .
P-SPEC    stage    pres  /  . . .
FURNACE    keyword=value
```

Keywords:

MODEL DUTY basis-OVFL TEMP PRES

```
HEATERS    stage    duty / . . .
```

RUNBACK **stage** *keyword=value*

Keywords:

basis-FLOW **PA** **Q-STAGE**

STAGE-EFF **stage** **eff / . . .**
COMP-EFF **stage** **cid** **eff / . . .**
L2-STAGES **stage1** **stage2 / . . .**
SPEC **specno** **spectype** **value** *spec-keyword=value* *vary-keyword=value*

Spectypes:

basis-FRAC **basis-RECOV** **basis-FLOW** **basis-RATIO** **TEMP** **DUTY** **PROP** **PROP-DIFF** **basis-OVFL** **TBPT** **D86T** **D1160T** **VACT** **TBPWT** **D86WT** **D1160WT** **VACWT** **TBP-GAP** **D86-GAP** **TBPW-GAP** **D86W-GAP** **API** **RHOLSTD** **SG** **FLPT-API** **PRPT-API** **REFINDEX** **RVP-ASTM** **WAT**

Spec-keywords:

STREAMS **BASE-STREAMS** **STRIPPER** **STAGE** **BASE-STAGE** **PHASE** **BASE-PHASE** **PROPERTY** **BASE-PROPERTY** **COMPS** **BASE-COMPS** **PCT**

Vary-keywords:

VARYTYPE **VARY-STAGE** **VARY-STRIP** **VARY-PA** **VARY-STREAM**

T-EST **stage** **temp / . . .**
L-EST **stage** **flow / . . .**
V-EST **stage** **flow / . . .**
PDROP-SEC **secno** **stage1** **stage2** **pdrop / . . .**
STEFF-SEC **secno** **stage1** **stage2** **eff / . . .**
THERM-EFF **stage** **therm-eff / . . .**
THEFF-SEC **secno** **stage1** **stage2** **type** **therm-eff / . . .**
REPORT **reportopt-list**

Special reportopt-list:

NOPROFILE **COMPS** **NOHYDRAULIC** **NOENTH** **TARGET** **HYDANAL** **EXTHYD**

KEY-COMP **secno** **stage1** **stage2** **LIGHT-KEY=cid-list** **HEAVY-KEY=cid-list**
KEY-TOL **keyword=value**

Optional keywords:

KVAL-TOL **COMP-TOL** **SPF-LIMIT** **STG-SPAN** **EXCLD-KEY** **EXG-TREF**

CONVERGENCE *keyword=value*

Optional keywords:

STABLE-ITER **STABLE-METH** **TEFF-METHOD**

TRAY-REPORT *keyword=value*

Optional keywords:

TRAY-OPTION **FORMAT** **ORDER** **PROPERTIES** **WIDE**

INCL-TRAYS **stage1** **stage2 / . . .**
COND-HCURVE **curveno** *keyword=value*
REB-HCURVE **curveno** *keyword=value*

Optional keywords:

INDEP-VAR **LIST** **NPOINT** **INCR** **HEADING** **PROPERTIES** **PRES-PROFILE** **PDROP** **PRINT-PLOT** **HIGH-PRECISION** **LINES** **X-SCALE** **Y-SCALE** **WIDE** **GRID** **INTERPOLATE**

PSEUDO-STREAM **sid** **stage** **phase**
PLOT **plotno** **plot-list** **comp-plot=groupid-list** *keyword=value*

Plot list:

TEMP **PRES** **LRATE** **VRATE** **VL-RATIO**

Optional comp-plots:

X **Y** **KVL** **REL-VOL**

Optional keywords:

BASE-COMPS **BASIS** **ORDER** **PLOT-HEADING** **WIDE**

DIAGNOSTICS *keyword=value*

Keywords:

MAIN **OLVAR1** **OLVAR2** **CMBAL** **EMBAL** **DESIGN** **TERM** **TXYEST**

PUMPAROUND **paid** *keyword=value*

Keywords:

DRAW **RETURN** **TYPE** **basis-FLOW** **DUTY** **TEMP** **DELT** **QSTREAM-IN** **QSTREAM-OUT**

PA-HCURVE **paid** **curveno** *keyword=value*

Optional keywords:

INDEP-VAR **LIST** **NPOINT** **INCR** **HEADING** **PROPERTIES** **PRES-PROFILE** **PDROP** **PRINT-PLOT** **HIGH-PRECISION** **LINES** **X-SCALE** **Y-SCALE** **WIDE** **GRID** **INTERPOLATE**

PA-PSEUDO-STREAM **paid** **sid** **STATE=value**
STRIPPER **stripid** *keyword=value*

Keywords:

NSTAGE **LDRAW** **VRETURN** **STEAM** **Q-REB** **PRODUCT** **STEAM:PROD** **basis-DRAW** **basis-B** **KEY-SELECT**

Optional keywords:

LRETURN **basis-LFLOW** **LR-DUTY** **LR-TEMP** **LR-DELT** **QREB-IN** **QREB-OUT** **QLR-IN** **QLR-OUT** **DP-STAGE** **DP-COL**

STR-PROP-SECTIONS **stripid** **stage1** **stage2** **opsetname** *keyword=value*

Keywords:

FREE-WATER **SOLU-WATER** **HENRY-COMPS**

```
STR-FEEDS    stripid    stage    basis-FLOW=value
STR-P-SPEC    stripid    stage    pres  / ...
STR-COMP-EFF    stripid    stage    cid    eff  / ...
STR-STAGE-EFF    stripid    stage    eff  / ...
STR-L2-STAGES    stripid    stage1    stage2  / ...
STR-T-EST    stripid    stage    temp  / ...
STR-L-EST    stripid    stage    flow  / ...
STR-V-EST    stripid    stage    flow  / ...
STR-PDROP-SEC    stripid    secno    stage1    stage2    pdrop  / ...
STR-STEFF-SEC    stripid    secno    stage1    stage2    eff  / ...
STR-THERM-EFF    stripid    stage    therm-eff  / ...
STR-THEFF-SEC    stripid    secno    stage1    stage2    type    therm-eff  / ...
STR-KEY-COMP    stripid    secno    stage1    stage2    LIGHT-KEY=cid-list    &
       HEAVY-KEY=cid-list
STR-KEY-TOL    stripid    keyword=value
```

Optional keywords:

KVAL-TOL COMP-TOL SPF-LIMIT STG-SPAN EXCLD-KEY EXG-TREF

```
STR-INCL-TRAYS    stripid    stage1    stage2  / ...
STR-REB-HCURVE    stripid    curveno    keyword=value
```

Optional keywords:

INDEP-VAR LIST NPOINT INCR HEADING PROPERTIES
PRES-PROFILE PDROP PRINT-PLOT HIGH-PRECISION LINES
X-SCALE Y-SCALE WIDE GRID INTERPOLATE

```
STR-PSEUDO-STREAM    stripid    sid    keyword=value
```

Keywords:

SOURCE STAGE PHASE DRAW STATE

```
STG-UTL    stage    utilityid
PA-UTL    pid    utilityid
STRPR-UTL    stripid    utilityid
UTILITIES    keyword=value
```

Optional keywords:

COND-UTIL REB-UTIL

Input Language Description for PETROFRAC

SUBOBJECTS

Use to enter a list of IDs for pumparounds and strippers. The IDs are character strings up to eight characters long. They are used for referencing pumparounds and strippers in other input statements. If you do not use the SUBOBJECTS statement, pumparounds and strippers are referenced by sequential integer numbers.

PUMPAROUND..... List of pumparound IDs

STRIPPER ..... List of stripper IDs

PROP-SECTIONS

Use to specify property options for main column segments. PROP-SECTIONS overrides the PROPERTIES sentence for a column segment. The input language for PROP-SECTIONS is the same as for the PROPERTIES sentence, except that PROP-SECTIONS requires that you specify the column segment. (For more information about the PROPERTIES sentence, see Chapter 11.)

Column initialization calculations are always performed using the specifications in the PROPERTIES sentence, regardless of the specifications given in the PROP-SECTIONS sentence. It is important that the property option in the PROPERTIES sentence gives reasonable property representation at the average condition of the column. Any option set name entered in the PROP-SECTIONS sentence must also be named in the PROPERTIES sentence. (For more information about specifying an option set, see Chapter 8.)

stage1..... Initial stage of a column segment

stage2..... Final stage of a column segment (Default=*stage1*)

opsetname..... Property option set to be used for column segment

PARAM

Use to enter configuration and operating specifications for the main column. The number of stages, pumparounds, and strippers are required. You can specify optional convergence parameters.

NSTAGE..... Number of stages in the main column, including condensers and reboilers. Must be greater than 1.

NPA..... Number of pumparounds

NSTRIP ..... Number of strippers

NSSTRIP ..... Total number of stages in strippers

EFF..... Type of efficiency specified using COMP-EFF or STAGE-EFF:

EFF=VAPOR	Vaporization efficiency
EFF=MURPHREE	Murphree efficiency (Default)

HYDRAULIC..... Flag to specify whether to perform calculations of hydraulic parameters (for example, flow parameter, reduced vapor throughput, tray loadings, and various transport properties): YES or NO. (Default=NO)

P-UPDATE ..... Update pressure profile during column sizing and rating calculations: YES or NO. (Default=NO)

P-FIX ..... Pressure update option: TOP or BOTTOM. Keep pressure at column top/bottom constant during pressure updating for column sizing and rating calculations. (Default=TOP)

DAMPING..... Damping factor, used to stabilize convergence when excessive oscillation is observed in the convergence behavior:

DAMPING=NONE	No damping (Default)
DAMPING=MILD	Mild level of damping
DAMPING=MEDIUM	Medium level of damping
DAMPING=SEVERE	Severe level of damping. You may need to increase the maximum number of iterations (keyword MAXIT) to achieve convergence

MAXIT..... Maximum number of iterations (Default=25)

TOL ..... Convergence tolerance (Default=1×10^{-4})

METHOD..... Convergence methods:

METHOD=SCHUBERT	Schubert quasi-Newton method with Powell's dogleg stabilization strategy (Default)
METHOD=BROYDEN	Broyden quasi-Newton method

ALGORITHM ..... Algorithm convergence options:

ALGORITHM=STANDARD	Normal algorithm. Recommended for most two-phase columns. May also be used to perform free water calculations in the condenser. (Default)
ALGORITHM=SUM-RATES	Recommended for petroleum and petrochemical applications involving wide-boiling mixtures and may components and/or design specifications. Free water calculations are allowed in the condenser.

THERM-EFF ..... Type of thermal efficiency specified using THERM-EFF or THEFF-SEC sentences. Thermal efficiencies allow deviation from thermal equilibrium on a stage.

THERM-EFF=VAPOR	Vapor efficiency (Default)
THERM-EFF=LIQUID	Liquid efficiency

INIT-OPTION ..... Initialization options:

INIT-OPTION=STANDARD	Standard initialization using composite feed flash
INIT-OPTION=CRUDE	Special initialization method for petroleum applications (Default)

DSMETH ..... Design specification convergence method:

DSMETH=SIMULT	Simultaneous method (Default)
DSMETH=NESTED	Nested-iteration method

FLASH-MAXIT ..... Maximum number of feed flash iterations (Default=50)

FLASH-TOL..... Feed flash tolerance (Default=$1x10^{-4}$)

FLOW-RF2..... Flow fraction to control liquid and vapor flow variable changes during iterations (Default=1.0)

HMODEL2..... Temperature dependence option for local enthalpy departure model:

HMODEL2=NO-TEMP	No temperature dependence
HMODEL2=TEMP	Temperature dependence term is computed initially, and is then kept constant
HMODEL2=UPDATE	Temperature dependence term is updated every iteration

(Default is selected based on column specifications)

INCL-THEFF ..... Switch for inclusion of thermal efficiency specifications during sequential calculation passes

INCL-THEFF=YES	Thermal efficiency specifications are honored for both sequential and equation-oriented passes (Default)
INCL-THEFF=NO	Thermal efficiency specifications are ignored during sequential calculation passes but are honored during equation-oriented passes

KBBMAX..... Maximum allowable slope value for local average K-value model (Default =-500)

KMODEL..... Weighting option for local average K-value model:

KMODEL=Y	Vapor mole fraction
KMODEL=X	Liquid mole fraction
KMODEL=K	Vapor fraction/(1+K-value)

(Default is selected based on column specifications)

MAX-BROY ..... Maximum number of variables converged by the Broyden method in the outside loop. You should not increase MAX-BROY beyond 900. (Default=200)

MAXIL ..... Maximum number of inside loop iterations per outside loop (Default=10)

MAXIO ..... Maximum number of inside loop iterations before activating Newton's method. Used only when thermal efficiency specifications exist.

MAXIP ..... Maximum number of initialization calculation passes. Default is selected based on column specifications.

NHOMOTOPY ..... Number of homotopy steps. Use only when thermal efficiency specifications exist and are honored during sequential calculation passes. (Default=1)

PROD-FLASH ..... Flash type for product stream in PROP-SET and recycle stream convergence calculations:

PROD-FLASH=PV	Flash with stream pressure and vapor fraction as specifications
PROD-FLASH=TP	Flash with stream temperature and pressure as specifications

(Default is selected based on column specifications)

QMAXBWIL ..... Maximum value of bounded Wegstein acceleration parameter for inside loop convergence (Default=0.5)

QMAXBWOL ..... Maximum value of bounded Wegstein acceleration parameter for outside loop convergence (Default=0.5)

QMINBWIL ..... Minimum value of bounded Wegstein acceleration parameter for inside loop convergence (Default=0)

QMINBWOL ..... Minimum value of bounded Wegstein acceleration parameter for outside loop convergence (Default=0)

RMSOL0 ..... Threshold value of outside loop RMS error that must be achieved before design specification iterations are performed (Default=1.0)

RMSOL1 ..... Threshold value of outside loop RMS error below which Broyden method is used for selected variables (Default=0.01)

STOR-FACTOR ..... Storage multiplier to override the internally calculated workspace requirement when thermal efficiency specifications exist and are honored during sequential calculation passes (Default=1.0)

TOLIL0 ..... Initial value of inside loop tolerance (Default=0.01)

TOLILFAC ..... Ratio of inside loop tolerance to outside loop RMS error (Default=0.05)

TOLILMIN ..... Minimum value of inside loop tolerance (Default=3×10^{-6})

JMETH ..... Jacobian calculation method

JMETH=INIT	Jacobian matrix is computed initially by numerical perturbation, then updated by the Broyden method (Default)
JMETH=RMSOL	Jacobian matrix is computed by numerical perturbation until outside loop RMS error is below RMSOLJ. Then the matrix is updated by the Broyden method.

RMSOLJ..... Value of the outside loop error below which the inside loop Jacobian matrix is updated by the Broyden method (Default=0.01)

TOLILO ..... Convergence tolerance for initialization iterations. Use only when thermal efficiency specifications exist. (Default=$1x10^{-3}$)

COL-SPECS

Use to enter configuration and operating specifications for the main column. Substitute MOLE, MASS, or STDVOL for the word *basis* in the following specifications. Table 15.5 lists the valid column specification combinations.

CONDENSER.....	**CONDENSER=TOTAL**	Total condenser
	CONDENSER= SUBCOOLED	Subcooled condenser
	CONDENSER=PARTIAL-V	Partial condenser with vapor distillate
	CONDENSER= PARTIAL-VL	Partial condenser with both vapor and liquid distillates
	CONDENSER= NONE-TOPPA	No condenser. Reflux is generated by a pumparound to the top stage.
	CONDENSER= NONE-TOPFEED	No condenser. Reflux is generated by an external feed to the top stage.
REBOILER	**REBOILER= NONE-BOTFEED**	No reboiler. Boilup is provided by an external feed to the bottom stage. (Default)
	REBOILER=NONE-BOTPA	No reboiler. Boilup is provided by a pumparound to the bottom stage.
	REBOILER=KETTLE	Kettle reboiler

T1 ..... Condenser temperature. Allowed only when CONDENSER=SUBCOOLED or PARTIAL-VL.

basis-RR ..... Reflux ratio, excluding free-water

basis-L1 ..... Reflux rate, excluding free-water

basis-D ..... Distillate flow rate, excluding free-water

basis-B..... Bottoms flow rate

Q-COND ..... Condenser (or top stage) duty

Q-REB ..... Reboiler (or bottom stage) duty

DP-STAGE ..... Pressure drop per stage

DP-COL ..... Pressure drop for column

basis-DV:D..... Distillate vapor fraction. DV:D=DV/D where DV is the distillate vapor flow rate and D is the total distillate flow rate, excluding any free-water.

STEAM..... ID of optional stripping steam feed

STEAM:PROD..... Optional stripping steam to bottom product ratio, entered in mass flow of steam per barrel of product. If STEAM:PROD is entered, PETROFRAC will override the flow specification given in the STREAM paragraph.

DEGSUB ..... Degrees of subcooling in the condenser. Allowed only when CONDENSER=SUBCOOLED.

KEY-SELECT ..... Method for selection of light and heavy key components for column targeting analysis. Specify KEY-SELECT if TARGET or HYDANAL report option is selected in the REPORT sentence.

KEY-SELECT=USER	Use light and heavy key components specified in KEY-COMP sentence.

KEY-SELECT= SPLIT-FRACTION	Select the light and heavy key components on the basis of component split-fractions in column product streams. This method is best suited for sharp or near-sharp splits.
KEY-SELECT=K-VALUE	Select the light and heavy key components on the basis of component K-values. This method is best suited for sloppy splits. (Default)
KEY-SELECT= COMP-PROFILE	Select the light and heavy key components on the basis of composition profiles. In principle, this method is similar to KEY-SELECT= K-VALUE. It is best suited for sloppy splits and it is, in general, inferior to KEY-SELECT= K-VALUE.

FEEDS Use to enter inlet material and heat stream locations, and feed conventions for material streams.

sid..... Stream ID

stage..... Stage number

feed-conv.....

ABOVE-STAGE	Introduces feed between stages, above designated stage (Default)
ON-STAGE	Introduces feed on designated stage
ON-STAGE-VAP	Introduces vapor phase feed on designated stage
ON-STAGE-LIQ	Introduces liquid phase feed on designated stage
FURNACE	Introduces feed to furnace attached to the specified stage

PRODUCTS Use to enter outlet stream locations, phases, and flows. When L2-STAGES is not specified, *phase*=W is allowed for stage 1 (condenser) only. When L2-STAGES is specified, *phase*=W is allowed for any stage included in L2-STAGES.

sid..... Stream ID

stage..... Stage number

phase..... Product phase:

L	Liquid
W	Water decant
V	Vapor
TL	Total drawoff of stage liquid
TV	Total drawoff of stage vapor

(Default is selected based on the product stream specifications)

basis-FLOW..... Flow rate for side products on MOLE, MASS, or STDVOL basis. Not allowed when *phase*=W. When *phase* is TL or TV, specified value is treated as initial estimate only.

P-SPEC Use to enter the column pressure profile.

stage..... Stage number

pres ..... Pressure

FURNACE Use to enter optional feed furnace specifications.

MODEL .....

MODEL=FLASH	Single-stage flash
MODEL=FLASH-BYPASS	Single-stage flash with the overflash bypassed back to the furnace
MODEL=HEATER	Stage heat duty on the feed stage (Default)

DUTY..... Furnace heat duty

basis-OVFL..... Fractional overflash (liquid runback from the stage above the feed stage/furnace feed flow) on MOLE, MASS, or STDVOL basis

TEMP..... Furnace temperature.

PRES..... Furnace pressure. Required when MODEL=FLASH or FLASH-BYPASS.

HEATERS

Use to enter the heater stage locations and duties. You can use inlet heat streams in place of HEATERS specifications.

stage..... Stage number

duty..... Heat duty

RUNBACK

Use to specify the flow rate of liquid runback from any stage. You must allow the flow of a pumparound or the duty of a heater to vary to satisfy the flow specification.

stage..... Stage number for specified flow

basis-FLOW..... Liquid flow rate

PA..... ID of a pumparound whose flow is to be manipulated. You cannot enter PA if you specified Q-STAGE.

Q-STAGE..... Stage number of heater whose duty is to be manipulated. You cannot enter Q-STAGE if you specified PA.

STAGE-EFF

Use to enter stage efficiency. These efficiencies are applied to each component on the stage. You cannot use STAGE-EFF if you specified COMP-EFF or STEFF-SEC. The efficiency type is specified by keyword EFF in the PARAM statement.

stage..... Stage number. Enter stage number and efficiency for one or more stages. Intermediate stage efficiencies are calculated by linear interpolation.

eff..... Efficiency (Default=1)

COMP-EFF

Use to enter component efficiency. You cannot use COMP-EFF if you specified STAGE-EFF or STEFF-SEC. The efficiency type is specified by keyword EFF in the PARAM statement.

stage..... Stage number. Enter stage number and efficiency for one or more stages. Intermediate stage efficiencies are calculated by linear interpolation.

cid..... Component ID

eff..... Efficiency for an individual component (Default=1)

L2-STAGES

Use to indicate a column segment to be tested for water phase, when FREE-WATER=YES is specified for the block. By default the top stage is tested for a free-water phase.

stage1..... Initial stage of a column segment to be tested for the presence of a free-water phase

stage2..... Final stage of a column segment to be tested for the presence of a free-water phase

SPEC

Use to enter design specifications. For each design specification, you must define the associated manipulated variable. The specified value for the manipulated variable is treated as an initial guess. Substitute MOLE, MASS, or STDVOL for the word *basis.*

specno..... Design specification number

spectype..... Design specification type:

basis-FRAC	Purity of a product stream (specified by STREAMS) or an internal stream (specified by STAGE and PHASE) FRAC = $\Sigma x_i / \Sigma x_j$ Where: x = Component fraction i = Component in the COMPS list j = Component in the BASE-COMPS list. The default for BASE-COMPS is all components $\Sigma x_j = 1$.
basis-RECOV	Component recovery : RECOV = $\Sigma\Sigma f_{ik} / \Sigma\Sigma f_{ij}$ Where: f = Component flow rate i = Component in the COMPS list j = Product stream in the STREAMS list k = Feed stream in the BASE-STREAMS list. The default for BASE-STREAMS is all feed streams.
basis-FLOW	Flow rate of a group of components (specified by COMPS) in a set of product streams (specified by STREAMS) or an internal stream (specified by STAGE and PHASE). The default for COMPS is all components.
basis-RATIO	RATIO= $\Sigma\Sigma f_{i1} / \Sigma\Sigma f_{j2}$ (BASE-STAGE specified) or $\Sigma\Sigma f_{i1} / \Sigma\Sigma f_{jk}$ (BASE-STREAMS specified or default)

For basis-RATIO:

i = Component in the COMPS list

j = Component in the BASE-COMPS list

k = Stream in the BASE-STREAMS list

f_{i1} = Component *i* flow rate in an internal stream specified by STAGE and PHASE

f_{j2} = Component *j* flow rate in an internal stream specified by BASE-STAGE and BASE-PHASE

f_{jk} = Component *j* flow rate in a feed or product stream in the BASE-STREAMS list. (The BASE-STREAMS list cannot mix feed and product streams.)

The default for COMPS and BASE-COMPS is all components, and the default for BASE-STREAMS is all feed streams.

TEMP	Temperature on a given STAGE of the column
DUTY	Heat duty of a stage (specified by STAGE).
PROP	Property value, as specified by PROPERTY, for a product stream (specified by STREAMS) or an internal stream (specified by STAGE and the property phase qualifier in the corresponding PROP-SET paragraph).
PROP-DIFF	Property value minus base property value, as specified by PROPERTY and BASE-PROPERTY. PROPERTY is the property of a product stream (specified by STREAMS) or of an internal stream (specified by STAGE and the phase qualifier in the corresponding PROP-SET paragraph). BASE-PROPERTY is the property of a product stream (specified by BASE-STREAMS) or of an internal stream (specified by BASE-STAGE and the phase qualifier in the corresponding PROP-SET paragraph).

basis-OVFL	Fractional feed overflash
TBPT	True boiling point temperature (dry, liquid volume basis) of a product stream (specified by STREAMS)
D86T	ASTM D86 temperature (dry, liquid volume basis) of a product stream (specified by STREAMS)
D1160T	ASTM D1160 temperature at 10 mm Hg (dry, liquid volume basis) of a product stream (specified by STREAMS)
VACT	Vacuum temperature at 10 mm Hg (dry, liquid volume basis) of a product stream (specified by STREAMS)
TBPWT	True boiling point temperature (dry, weight basis) of a product stream (specified by STREAMS)
D86WT	ASTM D86 temperature (dry, weight basis) of a product stream (specified by STREAMS)
D1160WT	ASTM D1160 temperature at 10 mm Hg (dry, weight basis) of a product stream (specified by STREAMS)
VACWT	Vacuum temperature at 10 mm Hg (dry, weight basis) of a product stream (specified by STREAMS)
TBP-GAP	Difference between 5% TBP temperature of a product stream (STREAMS) and 95% TBP temperature of a product stream (BASE-STREAMS) (dry, liquid volume basis)
D86-GAP	Difference between 5% D86 temperature of a product stream (STREAMS) and 95% D86 temperature of a product stream (BASE-STREAMS) (dry, liquid volume basis)
TBPW-GAP	Difference between 5% TBP temperature of a product stream (STREAMS) and 95% TBP temperature of a product stream (BASE-STREAMS) (dry, weight basis)
D86W-GAP	Difference between 5% D86 temperature of a product stream (STREAMS) and 95% D86 temperature of a product stream (BASE-STREAMS) (dry, weight basis)
API	API gravity (dry basis) of a product stream (specified by STREAMS)
RHOLSTD	Standard liquid density (dry basis) of a product stream (specified by STREAMS)
SG	Specific gravity (dry basis) of a product stream (specified by STREAMS)
FLPT-API	Flash point computed from the API correlation (dry basis) of a product stream (specified by STREAMS)
PRPT-API	Pour point computed from the API correlation (dry basis) of a product stream (specified by STREAMS)
REFINDEX	Refractive index (dry basis) of a product stream (specified by STREAMS)
RVP-ASTM	Reid vapor pressure computed from ASTM procedure (dry basis) of a product stream (specified by STREAMS)
WAT	Watson UOP K-factor (dry basis) of a product stream (specified by STREAMS)

value..... Desired value of the design specification

STREAMS	List of the stream IDs	
BASE-STREAMS	List of streams IDs	
STRIPPER	Stripper ID	
STAGE	Stage number	
BASE-STAGE	Stage number	
PHASE	**PHASE=L**	Liquid (Default)
	PHASE=V	Vapor
BASE-PHASE	**BASE-PHASE=L**	Liquid
	BASE-PHASE=V	Vapor (Default)
PROPERTY	ID of a property set defined by a PROP-SET paragraph consisting of a scalar property. (See Chapter 41.)	
BASE-PROPERTY	ID of a property set defined by a PROP-SET paragraph consisting of a scalar property. (See Chapter 41.)	
COMPS	List of component IDs	
BASE-COMPS	List of component IDs (Default=all components)	
PCT	Liquid volume percent for *spectypes*: TBPT, D86T, D1160T, or VACT. Liquid weight percent for *spectypes*: TBPWT, D86WT, D1160WT, or VACWT.	
VARYTYPE	Manipulated variable type. You must enter the initial estimate in the corresponding COL-SPECS, STRIPPER, or PUMPAROUND statements:	
	VARYTYPE=basis-LPROD	Liquid sidestream product flow rate. You must also specify STAGE
	VARYTYPE=basis-VPROD	Vapor sidestream product flow rate. You must also specify STAGE
	VARYTYPE=DUTY	External heater duty of the column. You must also specify STAGE
	VARYTYPE=basis-D	Distillate flow, excluding free-water when FREE-WATER=YES. Distillate flow includes both vapor and liquid distillates.
	VARYTYPE=basis-L1	Reflux rate, excluding free-water if FREE-WATER=YES
	VARYTYPE=basis-B	Main column or stripper bottoms flow rate
	VARYTYPE=basis-RR	Reflux ratio (L1/D), excluding free-water when FREE-WATER=YES
	VARYTYPE=Q-COND	Condenser (or top stage) heat duty
	VARYTYPE=Q-REB	Main column or stripper reboiler heat duty
	VARYTYPE= basis-RUNBACK	Main column stage liquid flow
	VARYTYPE=T1	Condenser (or top stage) temperature
	VARYTYPE=FURN-TEMP	Furnace temperature
	VARYTYPE=FURN-DUTY	Furnace heat duty
	VARYTYPE= basis-PA-FLOW	Pumparound stream flow
	VARYTYPE=PA-TEMP	Pumparound stream temperature
	VARYTYPE=PA-DELT	Pumparound stream temperature change
	VARYTYPE=PA-DUTY	Pumparound stream duty
	VARYTYPE=FEED-FLOW	Feed mass flow rate

VARY-STAGE ..... Main column stage number. Required when VARYTYPE=LPROD, VPROD, and DUTY.

VARY-STRIP ..... Stripper ID (optional when VARYTYPE=B and QN)

VARY-PA ..... Pumparound ID. Required when VARYTYPE=PA-FLOW, PA-TEMP, PA-DELT, and PA-DUTY.

VARY-STREAM..... Feed stream ID. Required when VARYTYPE=FEED-FLOW.

T-EST

Use to enter an initial estimate of the column temperature profile. If you do not give a T-EST sentence, an initial profile is generated by PETROFRAC.

stage..... Stage number

temp ..... Temperature

L-EST
V-EST

Use to enter initial estimates of liquid and vapor flow profiles. The flow entered is the total flow of the respective phase, including any portions withdrawn as products. If you do not give L-EST or V-EST, an initial profile is generated by PETROFRAC.

stage..... Stage number

flow ..... Molar flow rate

PDROP-SEC

Use to enter pressure drop across a section of the column. You must also specify the pressure for *stage1* in the P-SPEC sentence. You cannot use PDROP-SEC if you specify DP-STAGE, DP-COL, or P-SPEC for any other stage.

secno ..... Section number

stage1..... Stage number for initial stage of column segment

stage2..... Stage number for final stage of column segment

pdrop ..... Pressure drop across section

STEFF-SEC

Use to enter stage Murphree or vaporization efficiencies for a column section. These efficiencies are applied to each component on each stage of the column section. Specify the efficiency type by using EFF in the PARAM sentence. You cannot use STEFF-SEC if you specified COMP-EFF or STAGE-EFF.

secno ..... Section number

stage1..... Stage number for initial stage of column segment

stage2..... Stage number for final stage of column segment

eff ..... Efficiency (Default=1)

THERM-EFF

Use to enter thermal efficiency. These efficiencies allow deviation from thermal equilibrium on a stage. Specify the type of thermal efficiency by using THERM-EFF in the PARAM sentence. You cannot use THERM-EFF if you specified THEFF-SEC.

stage..... Stage number

therm-eff ..... Thermal efficiency (Default=1)

THEFF-SEC

Use to enter thermal efficiencies across a section of the column. These efficiencies allow deviation from thermal equilibrium on column stages. You cannot use THEFF-SEC if you specified THERM-EFF.

secno ..... Section number

stage1..... Stage number for initial stage of column segment

stage2..... Stage number for final stage of column segment

type ..... Type of thermal efficiency:

VAPOR	Vapor efficiency

	LIQUID	Liquid efficiency

therm-eff ..... Thermal efficiency (Default=1)

REPORT

Use to override the default report options. You can use the standard REPORT options for use within a block (see Chapter 11) for PETROFRAC.

reportopt ..... Standard block report options (see Chapter 11), in addition to the following:

NOPROFILE	Suppress the stagewise profiles of temperature, operating pressure, flows, enthalpies, and duties for this block
COMPS	Include the mole fraction and K-value profiles for this block
NOHYDRAULIC	Suppress the hydraulic parameters reported for this block
NOENTH	Suppress the enthalpy profile for this block
TARGET	Include column targeting thermal analysis results
HYDANAL	Include column targeting hydraulic analysis results
EXTHYD	Include extended hydraulic parameter report. Use only when NOHYDRAULIC report option is not selected or when HYDRAULIC=YES in the PARAM sentence.

KEY-COMP

Use to specify light and heavy key components for column targeting analysis. Use only when TARGET and/or HYDANAL report option is selected and KEY-SELECT=USER in the COL-SPECS sentence for the main column.

secno ..... Section number for key component specification

stage1..... Stage number for the initial stage of the section

stage2..... Stage number for the final stage of the section

LIGHT-KEY ..... List of light key components

HEAVY-KEY ..... List of heavy key components

KEY-TOL

Use to specify tolerances and other parameters for light and heavy key component selection methods other than KEY-SELECT=USER and for exergy loss calculations. Use only when TARGET and/or HYDANAL report option is selected.

KVAL-TOL..... Tolerance on component K-values. Specify when KEY-SELECT= K-VALUE or SPLIT-FRACTION. (Default=$1x10^{-5}$)

COMP-TOL..... Tolerance on component mole-fractions. Specify when KEY-SELECT=
K-VALUE, SPLIT-FRACTION, or COMP-PROFILE. (Default=$1x10^{-6}$)

SPF-LIMIT..... Minimum value of component split-fractions, in the top and the bottom products of a column section, necessary for key component selection. Specify when KEY-SELECT=SPLIT-FRACTION. (Default=0.9)

STG-SPAN ..... Stage span for computing composition profiles. Specify when KEY-SELECT=COMP-PROFILE. (Default=2)

EXCLD-KEY..... List of components to be excluded from key component selection. Specify when KEY-SELECT=K-VALUE, SPLIT-FRACTION, or COMP-PROFILE.

EXG-TREF..... Reference temperature for exergy loss calculations (Default=298.15 K)

CONVERGENCE	Use to specify advanced convergence parameters		
	STABLE-ITER	Initial number of iterations over which the steps are damped using a stabilization method. Use when thermal efficiencies are specified.	
	STABLE-METH	Stabilization method. Use when thermal efficiencies are specified.	
		STABLE-METH=DOGLEG	Powell's dogleg strategy
		STABLE-METH=LINE-SEARCH	One-dimensional line search (Default)
	TEFF-METHOD	Convergence method for thermal efficiency calculations	
		TEFF-METHOD=NEWTON	Newton's method (Default)
		TEFF-METHOD=SCHUBERT	Schubert quasi-Newton method
TRAY-REPORT	Use to specify the format of the report and additional tray properties to be reported (in addition to the flows, temperatures, pressures, enthalpies, and duties printed in the standard report).		
	TRAY-OPTION	**TRAY-OPTION=BRIEF**	Reports the stages that have feeds, products, heaters, maximum and minimum flows, and the stages immediately above and below those stages (Default)
		TRAY-OPTION=INCL-TRAY	Reports the stages specified in the INCL-TRAYS statement
		TRAY-OPTION=ALL-TRAYS	Reports all trays in the column
	FORMAT	**FORMAT=PROFILE**	Prints tabular column profiles (Default)
		FORMAT=STAGE	Prints individual stage reports for each stage
		FORMAT=COMBINED	Prints both tabular column profiles and individual stage reports
	ORDER	Tray numbering order. Use for report only.	
		ORDER=TOP-DOWN	Number of stages from top down in report (Default)
		ORDER=BOTTOM-UP	Number of stages from bottom up in report
	PROPERTIES	List of properties set IDs	
	WIDE	Report width option	
		WIDE=YES	Produces wide (132 columns) reports (Default)
		WIDE=NO	Produces standard (80 columns) reports
INCL-TRAYS	Use to designate trays to be included in the report when TRAY-OPTION=INCL-TRAYS.		
	stage1	Stage number of initial stage of column segment to be reported	
	stage2	Stage number of final stage of column segment to be reported (Default=*stage1*)	
COND-HCURVE, REB-HCURVE	Use to generate heating/cooling curve tables for the condenser or reboiler of the column. If you specify efficiency for a condenser (or reboiler) using COMP-EFF or STAGE-EFF, cooling (or heating) curves calculated for that condenser (or reboiler) will not be consistent with column results. See Chapter 11 for a description of input keywords.		
PSEUDO-STREAM	Use to define outlet streams as pseudostreams and to enter their locations and phases.		
	sid	Stream ID	
	stage	Stage number	
	phase	**L**	Stage liquid excluding any liquid sidedraw (Default)
		V	Stage vapor excluding any vapor sidedraw
		TL	Total stage liquid

	TV	Total stage vapor

PLOT

Use to generate stagewise plots of column profiles. You can report properties on a MOLE, MASS, or STDVOL basis.

plotno ..... Plot number

plot-list ..... List of non-component-dependent properties to be plotted:

TEMP	Temperature
PRES	Pressure
LRATE	Liquid flow rate
VRATE	Vapor flow rate
VL-RATIO	Vapor flow rate/liquid flow rate

comp-plot ..... Keyword for component-dependent property to be plotted:

X,Y	Fraction of the components and/or component groups listed are plotted
KVL	K-values of the components and/or component groups listed are plotted
REL-VOL	Relative volatilities of the components and/or component listed are plotted. You must also specify BASE-COMP. When a component group ID is specified, $$REL-VOL = \frac{\Sigma y_i / \Sigma x_i}{(y/x)_{BASE-COMP}}$$

groupid-list ..... List of component IDs and/or component group IDs

BASE-COMP..... Component ID of base component for relative volatility calculations. (Use with REL-VOL keyword.)

BASIS	**BASIS=MOLE**	Plotted results are on a mole basis (Default)
	BASIS=MASS	Plotted results are on a mass basis
	BASIS=STDVOL	Plotted results are on a standard-liquid- volume basis
ORDER	**ORDER=TOP-DOWN**	Number of stages from top down in report (Default)
	ORDER=BOTTOM-UP	Number of stages from bottom up in report

PLOT-HEADING..... Heading up to 64 characters included in quotes, printed at the top of the print-plot

WIDE ..... Plot width option. Use to override default established by the PLOT-OPTIONS paragraph (See Chapter 46).

DIAGNOSTICS

Use to control the level of convergence diagnostics in the history and log files. You can enter a level between 0 and 10. The amount of diagnostics increases with each level.

MAIN ..... Controls printouts of initial/final profiles, inside/middle/outside loop iterations, and outside loop variables/functions in the history file (Default=4)

OLVAR1..... Controls initial local model parameter diagnostics in the history file (Default=4)

OLVAR2..... Controls local model parameter diagnostics for each outside loop in the history file (Default=4)

CMBAL ..... Controls component mass balance diagnostics for each inside loop in the history file (Default=4)

EMBAL..... Controls enthalpy balance diagnostics for each inside loop in the history file (Default=4)

DESIGN ..... Controls middle loop diagnostics in the history file (Default=4)

TERM ..... Controls printouts of inside/middle/outside loop iterations in the log file (Default=0)

TXYEST ..... Controls printouts of temperature and composition profile results in input estimate formats in the history file (Default=4)

PUMPAROUND

Use to enter pumparound connectivity and cooler/heater specifications. Pumparounds are associated with the main column. They can be total or partial drawoffs of the stage liquid flow. You must specify the draw and return stage locations for each pumparound.

paid ..... Pumparound ID

DRAW ..... Stage number of pumparound draw location. Must be greater than 1

RETURN ..... Stage number of pumparound return location

TYPE ..... Pumparound drawoff type:

TYPE=PARTIAL	Two of the following variables must be specified: basis-FLOW, DUTY, or TEMP (or DELT). (Default)
TYPE=TOTAL	One of the following variables must be specified: DUTY, TEMP or DELT.

basis-FLOW ..... Pumparound flow rate in MOLE, MASS, or STDVOL basis

DUTY ..... Heat duty for associated cooler/heater. Enter negative value for cooling, positive value for heating, 0 for no heating or cooling.

TEMP ..... Temperature of pumparound at associated cooler outlet. No phase change is assumed.

DELT ..... Temperature change from associated cooler inlet to outlet. Specified value must be negative.

QSTREAM-IN ..... Stream ID of inlet heat stream for the pumparound

QSTREAM-OUT ..... Stream ID of outlet heat stream for the pumparound

PA-HCURVE

Use to generate heating/cooling curve tables and plots for pumparound heater/cooler. You must specify pumparound ID. See Chapter 11 for a description of input keywords.

paid ..... Pumparound ID

PA-PSEUDO-STREAM

Use to associate a pseudostream with a pumparound. A pseudostream does not affect column calculations.

paid ..... Pumparound ID

sid ..... Stream ID

STATE ..... State condition for pseudostream:

STATE=OUTLET	At the outlet condition of pumparound heater/cooler (Default)
STATE=INLET	At the inlet condition of pumparound heater/cooler

STRIPPER

Use to enter connectivity and operating specifications for stripper. Substitute MOLE, MASS, or STDVOL for the word *basis*. By default the stripper connectivity consists of a liquid draw from the main column to the top stage of the stripper, and the stripper overhead return to the main column. Optionally, you can specify that a portion of the stripper bottom liquid returning to a stage in the main column.

stripid ..... Stripper ID

NSTAGE..... Number of stages, including reboiler. Reboiler, if present, is the bottom stage

LDRAW..... Stage number for liquid draw location in main column

VRETURN ..... Stage number of stripper overhead vapor return location in main column

STEAM..... Stripping steam stream ID. You cannot enter STEAM if you specified Q-REB.

Q-REB ..... Reboiler duty. You cannot enter Q-REB if you specified STEAM.

PRODUCT ..... Bottom product stream ID

STEAM:PROD..... Mass flow of steam per barrel of product. Use to override flow rate of steam specified in the STREAM paragraph.

basis-DRAW ..... Draw flow rate. You cannot enter basis-DRAW if you specified basis-B.

basis-B..... Bottom product flow rate. You cannot enter basis-B if you specified basis-DRAW.

LRETURN..... Stage number of optional stripper bottom liquid return location in main column

basis-LFLOW ..... Flow rate of optional bottom liquid return stream

LR-DUTY ..... Heat duty for associated heater/cooler for optional bottom liquid return stream. Enter negative value for cooling, positive value for heating, 0 for no heating or cooling.

LR-TEMP ..... Temperature of optional bottom liquid return stream at heater/cooler outlet. No phase change is assumed.

LR-DELT ..... Temperature change of optional bottom liquid return stream across associated heater/cooler inlet to outlet. Specified value must be negative.

QREB-IN ..... Stream ID of inlet heat stream at reboiler

QREB-OUT..... Stream ID of outlet heat stream at reboiler

QLR-IN..... Stream ID of inlet heat stream for optional bottom liquid return

QLR-OUT ..... Stream ID of outlet heat stream for optional bottom liquid return

DP-STAGE ..... Pressure drop per stage

DP-COL ..... Pressure drop for column

KEY-SELECT ..... Method for selection of light and heavy key components for column targeting analysis. Specify KEY-SELECT if TARGET or HYDANAL report option is selected in the REPORT sentence.

KEY-SELECT=USER	Use light and heavy key components specified in the STR-KEY-COMP sentence.
KEY-SELECT= SPLIT-FRACTION	Select the light and heavy key components on the basis of component split-fractions in stripper product streams. This method is best suited for sharp or near-sharp splits.
KEY-SELECT=K-VALUE	Select the light and heavy key components on the basis of component K-values. This method is best suited for sloppy splits. (Default)

KEY-SELECT= COMP-PROFILE	Select the light and heavy key components on the basis of composition profiles. In principle, this method is similar to KEY-SELECT= K-VALUE. It is best suited for sloppy splits and it is, in general, inferior to KEY-SELECT= K-VALUE.

STR-PROP-SECTIONS Use to enter property specifications for stripper column segments. STR-PROP-SECTIONS overrides the PROPERTIES sentence for a stripper column segment. The input language for STR-PROP-SECTIONS is the same as for the PROPERTIES sentence (see Chapter 11), except that STR-PROP-SECTIONS requires that you specify a stripper segment. Any option set specified in the STR-PROP-SECTIONS sentence must be named in the PROPERTIES sentence. (For more information about specifying an option set, see Chapter 8.)

stripid ..... Stripper ID

stage1..... Initial stage of a column segment using the specified property option set

stage2..... Final stage of a column segment using the specified property option set (Default=*stage1*)

opsetname..... Property option set to be used for stripper segment

STR-FEEDS Use to define optional feeds to the top stage of stripper, in addition to the draw specified in the STRIPPER sentence. Substitute MOLE, MASS, or STDVOL for the word *basis*.

stripid ..... Stripper ID

stage..... Stage number of additional liquid draw location in main column

basis-FLOW..... Draw flow rate

STR-P-SPEC Use to enter the stripper column pressure profile.

stripid ..... Stripper ID

stage..... Stage number

pres ..... Pressure

STR-COMP-EFF Use to enter component efficiency. You cannot use STR-COMP-EFF if you specified STR-STAGE-EFF or STR-STEFF-SEC. The efficiency type is defined by keyword EFF in the PARAM statement.

stripid ..... Stripper ID

stage..... Stage number. Enter stage number and efficiency for one or more stages. Intermediate stage efficiencies are calculated by linear interpolation.

cid..... Component ID

eff..... Efficiency for an individual component (Default=1)

STR-STAGE-EFF Use to enter stage efficiency. You cannot use STR-STAGE-EFF if you specified STR-COMP-EFF or STR-STEFF-SEC. The efficiency type is defined by keyword EFF in the PARAM statement.

stripid ..... Stripper ID

stage..... Stage number. Enter stage number and efficiency for one or more stages. Intermediate stage efficiencies are calculated by linear interpolation.

eff..... Efficiency (Default=1)

STR-L2-STAGES Use to indicate a stripper segment to be tested for the presence of a free-water phase, when FREE-WATER=YES is specified for the block.

stripid ..... Stripper ID

stage1..... Initial stage of a stripper segment to be tested for the presence of a free-water phase

stage2..... Final stage of a stripper segment to be tested for the presence of a free-water phase

STR-T-EST

Use to enter an initial estimate of the stripper column temperature profile. If you do not give a T-EST sentence, an initial profile is generated by PETROFRAC.

stripid ..... Stripper ID

stage..... Stage number

temp ..... Temperature

STR-L-EST, STR-V-EST

Use to enter initial estimates of liquid and vapor flow profiles. The flow entered is the total flow of the respective phase, including any portions withdrawn as products.

stripid ..... Stripper ID

stage..... Stage number

flow ..... Flow rate

STR-PDROP-SEC

Use to enter pressure drop across stripper sections. You must also specify the pressure for *stage1* in the STR-P-SPEC sentence. You cannot use STR-PDROP-SEC if you specify DP-STAGE, DP-COL, or STR-P-SPEC for any other stage.

stripid ..... Stripper ID

secno ..... Section number

stage1..... Stage number for initial stage of stripper segment

stage2..... Stage number for final stage of stripper segment

pdrop ..... Pressure drop across section

STR-STEFF-SEC

Use to enter stage Murphree or vaporization efficiencies for stripper sections. These efficiencies are applied to each component on each stage of the section. Specify the efficiency type by using EFF in the PARAM sentence. You cannot use STR-STEFF-SEC if you specified STR-COMP-EFF or STR-STAGE-EFF.

stripid ..... Stripper ID

secno ..... Section number

stage1..... Stage number for initial stage of stripper segment

stage2..... Stage number for final stage of stripper segment

eff..... Efficiency (Default=1)

STR-THERM-EFF

Use to enter thermal efficiency. These efficiencies allow deviation from thermal equilibrium on a stage. Only efficiencies of type VAPOR can be specified using STR-THERM-EFF. You cannot use STR-THERM-EFF if you specified STR-THEFF-SEC.

stripid ..... Stripper ID

stage..... Stage number

therm-eff ..... Thermal efficiency (Default=1)

STR-THEFF-SEC

Use to enter thermal efficiencies across stripper sections. These efficiencies allow deviation from thermal equilibrium. You cannot use STR-THEFF-SEC if you specified STR-THERM-EFF.

stripid ..... Stripper ID

secno ..... Section number

stage1..... Stage number for initial stage of stripper segment

stage2..... Stage number for final stage of stripper segment

type ..... Type of thermal efficiency:

VAPOR	Vapor efficiency
LIQUID	Liquid efficiency

therm-eff ..... Thermal efficiency (Default=1)

STR-KEY-COMP

Use to specify light and heavy key components for column targeting analysis. Use only when TARGET and/or HYDANAL report option is selected and KEY-SELECT=USER in the STRIPPER sentence for the column under consideration.

stripid ..... Stripper ID

secno ..... Section number for key component specification

stage1..... Stage number for the initial stage of the section

stage2..... Stage number for the final stage of the section

LIGHT-KEY ..... List of light key components

HEAVY-KEY ..... List of heavy key components

STR-KEY-TOL

Use to specify tolerances and other parameters for light and heavy key component selection methods other than KEY-SELECT=USER and for exergy loss calculations. Use only when TARGET and/or HYDANAL report option is selected.

stripid ..... Stripper ID

KVAL-TOL..... Tolerance on component K-values. Specify when KEY-SELECT= K-VALUE or SPLIT-FRACTION. (Default=$1x10^{-5}$)

COMP-TOL..... Tolerance on component mole-fractions. Specify when KEY-SELECT= K-VALUE, SPLIT-FRACTION, or COMP-PROFILE. (Default=$1x10^{-6}$)

SPF-LIMIT..... Minimum value of component split-fractions, in the top and the bottom products of a column section, necessary for key component selection. Specify when KEY-SELECT=SPLIT-FRACTION. (Default=0.9)

STG-SPAN ..... Stage span for computing composition profiles. Specify when KEY-SELECT=COMP-PROFILE. (Default=2)

EXCLD-KEY..... List of components to be excluded from key component selection. Specify when KEY-SELECT=K-VALUE, SPLIT-FRACTION, or COMP-PROFILE.

EXG-TREF..... Reference temperature for exergy loss calculations (Default=298.15 K)

STR-INCL-TRAYS

Use to designate trays to be included in the report when TRAY-OPTION=INCL-TRAYS. One STR-INCL-TRAYS statement is entered for each stripper for which tray reports are desired.

stripid ..... Stripper ID

stage1..... Stage number of initial stage of a stripper column segment to be reported

stage2..... Stage number of final stage of a stripper column segment to be reported (Default=*stage1*)

STR-REB-HCURVE

Use to generate cooling curve tables and plots for the stripper reboiler. You must specify stripper ID. See Chapter 11 for a description of input keywords.

stripid ..... Stripper ID

STR-PSEUDO-STREAM Use to define pseudo streams for stripper streams.

stripid ..... Stripper ID

sid..... Stream ID

SOURCE ..... Source for the pseudostream:

SOURCE=OVERHEAD	Stripper vapor overhead stream
SOURCE=FEED	Stripper top feed stream
SOURCE=STAGE-FLOW	Stripper stage liquid/vapor stream (Default)
SOURCE=L-RETURN	Stripper bottom liquid return stream

STAGE ..... Stripper stage number, required if SOURCE=STAGE-FLOW

PHASE..... Withdrawal phase, required when SOURCE=STAGE-FLOW:

PHASE=L	Stage liquid excluding any liquid sidedraw (Default)
PHASE=V	Stage vapor excluding any vapor sidedraw
PHASE=TL	Total stage liquid
PHASE=TV	Total stage vapor

DRAW ..... Main column draw stage, required when SOURCE=FEED

STATE ..... State condition for L-RETURN pseudostream, required when SOURCE=L-RETURN:

STATE=OUTLET	At the outlet condition of heater/cooler (Default)
STATE=INLET	At the inlet condition of heater/cooler

STG-UTL Use to specify optional utilities to provide heating or cooling duty for stage heaters and coolers.

stage..... Stage number.

utilityid ..... Utility ID.

PA-UTL Use to specify optional utilities to provide heating or cooling duty for pumparounds.

pid ..... Pumparound ID.

utilityid ..... Utility ID.

STRPR-UTL Use to specify optional utilities to provide heating or cooling duty for strippers.

stripid ..... Stripper ID.

utilityid ..... Utility ID.

UTILITIES Use to specify optional utilities to provide heating or cooling duty for condenser and reboiler.

COND-UTIL ..... Utility ID for condenser.

REB-UTIL ..... Utility ID for reboiler.

Accessing Variables in PETROFRAC

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	ID2	ID3
PARAM	NPA, NSTRIP, NSSTRIP, NSTAGE	—	—	—
COL-SPECS	T1, basis-DV:D,basis-B, basis-D, basis-L1,basis-RR, Q-COND, Q-REB, STEAM:PROD,DP-STAGE, DP-COL	—	—	—
FEEDS	STAGE	sid	—	—
PRODUCTS	STAGE, basis-FLOW	sid	—	—
P-SPEC	PRES	stage	—	—
FURNACE	DUTY, TEMP, PRES, basis-OVFL	—	—	—
HEATERS	DUTY	stage	—	—
RUNBACK	basis-FLOW, Q-STAGE,PA	stage	—	—
STAGE-EFF	EFF	stage	—	—
COMP-EFF	EFF	stage	cid	—
SPEC†	VALUE, STAGE, BASE-STAGE, PCT, VARY-STAGE	specno	—	—
T-EST	TEMP	stage	—	—
L-EST	FLOW	stage	—	—
V-EST	FLOW	stage	—	—
COND-HCURVE	INCR, NPOINT, PDROP	curveno	—	—
REB-HCURVE	INCR, NPOINT, PDROP	curveno	—	—
PSEUDO-STREAM	STAGE	sid	—	—
PUMPAROUND	DRAW, RETURN, basis-FLOW, TEMP, DELT, DUTY	paid	—	—
STRIPPER	NSTAGE, LDRAW, VRETURN, basis-FLOW, basis-DRAW, Q-REB, STEAM:PROD, LRETURN, basis-LFLOW, LR-TEMP, LR-DELT, LR-DUTY, DP-STAGE, DP-COL	stripid	—	—
STR-FEEDS	basis-FLOW	stripid	stage	—
STR-COMP-EFF	EFF	stripid	stage	cid
STR-STAGE-EFF	EFF	stripid	stage	—
STR-T-EST	TEMP	stripid	stage	—
STR-L-EST	FLOW	stripid	stage	—
STR-V-EST	FLOW	stripid	stage	—
STR-PSEUDO- STREAM	STAGE, DRAW	stripid	sid	—

† Accessed variables are in SI units.

Block Results

Description	Sentence	Variable	ID1	ID2	ID3
Main column condenser duty	RESULTS	COND-DUTY	—	—	—
Main column reboiler duty	RESULTS	REB-DUTY	—	—	—
Reflux ratio	RESULTS	RR	—	—	—
Boilup ratio	RESULTS	BR	—	—	—
Main column stage temperature	PROFILE	TEMP†	stage	—	—
Main column stage pressure	PROFILE	PRES†	stage	—	—
Main column liquid stage flow rate	PROFILE	LRATE†	stage	—	—
Main column liquid1 stage flow rate	PROFILE	L1RATE†	stage	—	—
Main column vapor stage flow rate	PROFILE	VRATE†	stage	—	—
Main column stage duty	PROFILE	DUTY†	stage	—	—
Main column liquid composition	COMPS	X†	cid	stage	—
Main column liquid1 composition	COMPS	X1†	cid	stage	—
Main column vapor composition	COMPS	Y†	cid	stage	—
Furnace duty	FURNACE-RESULTS	DUTY	—	—	—
Furnace temperature	FURNACE-RESULTS	TEMP	—	—	—
Furnace pressure	FURNACE-RESULTS	PRES	—	—	—
Furnace liquid flow rate	FURNACE-RESULTS	LRATE	—	—	—
Furnace vapor flow rate	FURNACE-RESULTS	VRATE	—	—	—
Furnace liquid composition	FURNACE-COMPS	X†	cid	—	—
Furnace vapor composition	FURNACE-COMPS	Y†	cid	—	—
Manipulated variable††	MAN-VARS	VALUE†	specno	—	—
Pumparound temperature	PA-RESULTS	TEMP	paid	—	—
Pumparound pressure	PA-RESULTS	PRES	paid	—	—
Pumparound duty	PA-RESULTS	DUTY	paid	—	—
Pumparound flow	PA-RESULTS	basis-FLOW	paid	—	—
Stripper stage temperature	STR-PROFILE	TEMP†	stripid	stage	—
Stripper stage pressure	STR-PROFILE	PRES†	stripid	stage	—
Stripper stage liquid flow rate	STR-PROFILE	LRATE†	stripid	stage	—
Stripper stage liquid1 flow rate	STR-PROFILE	L1RATE†	stripid	stage	—
Stripper stage vapor flow rate	STR-PROFILE	VRATE†	stripid	stage	—
Stripper stage duty	STR-PROFILE	DUTY†	stripid	stage	—
Stripper liquid composition	STR-COMPS	X†	cid	stage	stripid
Stripper liquid1 composition	STR-COMPS	X1†	cid	stage	stripid
Stripper vapor composition	STR-COMPS	Y†	cid	stage	stripid

† You can also access variables using the VECTOR-DEF sentence. See Chapter 29.

†† Accessed variables are in SI units.

Valid COL-SPECS Combinations

The allowed COL-SPECS combinations are indicated with an X in the following matrix:

Table 15.5 Column Specification Combinations

	RR	L1	Q-COND	Q-REB
D	X	X	X	X
B	X	X	X	X
Q-COND				X

If CONDENSER=NONE-TOPPA or NONE-TOPFEED, Q-COND is implicitly specified, and is used as one specification.

If REBOILER=NONE-BOTFEED or NONE-BOTPA, Q-REB is implicitly specified, and is used as one specification.

16 Column Design and Rating

This chapter describes the input language for the Aspen Plus column design and rating capabilities in RADFRAC, MULTIFRAC, and PETROFRAC.

The column design and rating capabilities in Aspen Plus allow you to request sizing, rating, and integrated pressure drop calculations for trayed and packed columns.

See also Chapter 15 for general input language used with these models, and Chapter 17 for input language used with RADFRAC for the RateSep rate-based distillation feature.

RADFRAC, MULTIFRAC and PETROFRAC

Input Language for RADFRAC

```
BLOCK    blockid    RADFRAC
                .
                .
                .
PARAM    keyword=value
```

Keywords for pressure drop calculations:

P-UPDATE P-FIX

```
                .
                .
                .
CONVERGENCE keyword=value
```

Keywords for tray sizing/rating:

KOCH-CORR NUTTER-CORR

```
TRAY-SIZE  secno  stage1  stage2  traytype  keyword=value
```

Keywords:

NPASS TRAY-SPACE FLOOD-FAC SYSFAC SLOT-AREA HOLE-AREA MIN-DIAM MIN-DCAREA OVER-DESIGN FLOOD-METH

```
TRAY-RATE  secno  stage1  stage2  traytype  keyword=value
```

Keywords:

NPASS TRAY-SPACE DIAM SYSFAC OVER-DESIGN EFF FLOOD-METH P-UPDATE DECK-THICK DC-OFC-WALL

Keywords for bubble cap trays:

CAP-DIAM NCAPS NROWS CAP-SPACE SKIRT-HT

Keywords for sieve trays:

HOLE-DIAM HOLE-AREA

Keywords for valve trays:

VALVE-TYPE VALVE-DEN NVALVES

Keywords for ballast trays:

VALVE-MAT VALVE-THICK

Keywords for float valve trays:

VALVE-LIFT DC-RTIME DC-EDGE

Optional keywords:

WEIR-HT-A WEIR-HT-B WEIR-HT-C WEIR-HT-D DC-CLEAR-SIDE DC-CLEAR-CTR DC-CLEAR-OFC DC-WTOP-SIDE DC-WTOP-CTR DC-WTOP-OFC DC-WBOT-SIDE DC-WBOT-CTR DC-WBOT-OFC DC-HT-SIDE DC-HT-CTR DC-HT-OFC

TRAY-RATE1 secno *keyword=value*

Keywords:

MAX-FLOOD-F MAX-DCBUP-F

PACK-SIZE secno stage1 stage2 packtype *keyword=value*

Keywords:

PACK-MAT PACK-SIZE VENDOR PACK-FAC SPAREA VOIDFR STICH1 STICH2 STICH3 SYSFAC OVER-DESIGN PACK-HT HETP PACK-THICK CS-APP CS-FLOOD CS-DESIGN DPMAX-SEC DPMAX-PACK DPMETH P-UPDATE

PACK-RATE secno stage1 stage2 packtype *keyword=value*

Keywords:

PACK-MAT PACK-SIZE VENDOR PACK-FAC SPAREA VOIDFR STICH1 STICH2 STICH3 SYSFAC OVER-DESIGN PACK-HT HETP PACK-THICK DIAM CS-FLOOD DPMETH P-UPDATE THETA

PACK-RATE1 secno MAX-FLOOD-F=value
SUBROUTINE *keyword=value*

Keywords:

TRAYSR PACKSR

TRSR-VECS *keyword=value*

Keywords:

TRNINT TRNREAL

TRSR-INT VALUE-LIST=values
TRSR-REAL VALUE-LIST=values
PCKSR-VECS *keyword=value*

Keywords:

PCKNINT PCKNREAL

PCKSR-INT VALUE-LIST=values
PCKSR-REAL VALUE-LIST=values

Input Language for MULTIFRAC

```
BLOCK    blockid    MULTIFRAC
                .
                .
                .
PARAM    keyword=value
```

Keywords for pressure drop calculations:

P-UPDATE P-FIX

```
                .
                .
                .
CONVERGENCE keyword=value
```

Keywords for tray sizing/rating:

KOCH-CORR NUTTER-CORR

```
TRAY-SIZE  secno  col  stage1  stage2  traytype  keyword=value
```

Keywords:

NPASS TRAY-SPACE FLOOD-FAC SYSFAC SLOT-AREA HOLE-AREA MIN-DIAM MIN-DCAREA OVER-DESIGN FLOOD-METH

```
TRAY-RATE  secno  col  stage1  stage2  traytype  keyword=value
```

Keywords:

NPASS TRAY-SPACE DIAM SYSFAC OVER-DESIGN EFF FLOOD-METH P-UPDATE DECK-THICK DC-OFC-WALL

Keywords for bubble cap trays:

CAP-DIAM NCAPS NROWS CAP-SPACE SKIRT-HT

Keywords for sieve trays:

HOLE-DIAM HOLE-AREA

Keywords for valve trays:

VALVE-TYPE VALVE-DEN NVALVES

Keywords for ballast trays:

VALVE-MAT VALVE-THICK

Keywords for float valve trays:

VALVE-LIFT DC-RTIME DC-EDGE

Optional keywords:

WEIR-HT-A WEIR-HT-B WEIR-HT-C WEIR-HT-D DC-CLEAR-SIDE DC-CLEAR-CTR DC-CLEAR-OFC DC-WTOP-SIDE DC-WTOP-CTR DC-WTOP-OFC DC-WBOT-SIDE DC-WBOT-CTR DC-WBOT-OFC DC-HT-SIDE DC-HT-CTR DC-HT-OFC

```
TRAY-RATE1  secno  keyword=value
```

Keywords:

MAX-FLOOD-F MAX-DCBUP-F

```
PACK-SIZE  secno  col  stage1  stage2  packtype  keyword=value
```

Keywords:

PACK-MAT PACK-SIZE VENDOR PACK-FAC SPAREA VOIDFR STICH1 STICH2 STICH3 SYSFAC OVER-DESIGN PACK-HT HETP PACK-THICK CS-APP CS-FLOOD CS-DESIGN DPMAX-SEC DPMAX-PACK DPMETH P-UPDATE

```
PACK-RATE  secno  col  stage1  stage2  packtype  keyword=value
```

Keywords:

PACK-MAT PACK-SIZE VENDOR PACK-FAC SPAREA VOIDFR STICH1 STICH2 STICH3 SYSFAC OVER-DESIGN PACK-HT HETP PACK-THICK DIAM CS-FLOOD DPMETH P-UPDATE

```
PACK-RATE1  secno  MAX-FLOOD-F=value
SUBROUTINE  keyword=value
```

Keywords:

TRAYSR PACKSR

```
TRSR-VECS  keyword=value
```

Keywords:

TRNINT TRNREAL

```
TRSR-INT  VALUE-LIST=values
TRSR-REAL  VALUE-LIST=values
PCKSR-VECS  keyword=value
```

Keywords:

PCKNINT PCKNREAL

```
PCKSR-INT  VALUE-LIST=values
PCKSR-REAL  VALUE-LIST=values
```

Input Language for PETROFRAC

```
BLOCK  blockid  PETROFRAC
          .
          .
          .
PARAM  keyword=value
```

Keywords for pressure drop calculations:

P-UPDATE P-FIX

```
          .
          .
          .
CONVERGENCE keyword=value
```

Keywords for tray sizing/rating:

KOCH-CORR NUTTER-CORR

TRAY-SIZE **secno** **stage1** **stage2** **traytype** *keyword=value*

Keywords:

NPASS TRAY-SPACE FLOOD-FAC SYSFAC SLOT-AREA HOLE-AREA MIN-DIAM MIN-DCAREA OVER-DESIGN FLOOD-METH

TRAY-RATE **secno** **stage1** **stage2** **traytype** *keyword=value*

Keywords:

NPASS TRAY-SPACE DIAM SYSFAC OVER-DESIGN EFF FLOOD-METH P-UPDATE DECK-THICK DC-OFC-WALL

Keywords for bubble cap trays:

CAP-DIAM NCAPS NROWS CAP-SPACE SKIRT-HT

Keywords for sieve trays:

HOLE-DIAM HOLE-AREA

Keywords for valve trays:

VALVE-TYPE VALVE-DEN NVALVES

Keywords for ballast trays:

VALVE-MAT VALVE-THICK

Keywords for float valve trays:

VALVE-LIFT DC-RTIME DC-EDGE

Optional keywords:

WEIR-HT-A WEIR-HT-B WEIR-HT-C WEIR-HT-D DC-CLEAR-SIDE DC-CLEAR-CTR DC-CLEAR-OFC DC-WTOP-SIDE DC-WTOP-CTR DC-WTOP-OFC DC-WBOT-SIDE DC-WBOT-CTR DC-WBOT-OFC DC-HT-SIDE DC-HT-CTR DC-HT-OFC

TRAY-RATE1 **secno** *keyword=value*

Keywords:

MAX-FLOOD-F MAX-DCBUP-F

PACK-SIZE **secno** **stage1** **stage2** **packtype** *keyword=value*

Keywords:

PACK-MAT PACK-SIZE VENDOR PACK-FAC SPAREA VOIDFR STICH1 STICH2 STICH3 SYSFAC OVER-DESIGN PACK-HT HETP PACK-THICK CS-APP CS-FLOOD CS-DESIGN DPMAX-SEC DPMAX-PACK DPMETH P-UPDATE

PACK-RATE **secno** **stage1** **stage2** **packtype** *keyword=value*

Keywords:

PACK-MAT PACK-SIZE VENDOR PACK-FAC SPAREA VOIDFR STICH1 STICH2 STICH3 SYSFAC OVER-DESIGN PACK-HT HETP PACK-THICK DIAM CS-FLOOD DPMETH P-UPDATE

PACK-RATE1 **secno** **MAX-FLOOD-F=value**

STR-TRAY-SIZE **stripid** **secno** **stage1** **stage2** **traytype** *keyword=value*

Keywords:

NPASS TRAY-SPACE FLOOD-FAC SYSFAC SLOT-AREA HOLE-AREA MIN-DIAM MIN-DCAREA OVER-DESIGN FLOOD-METH

STR-TRAY-RATE **stripid** **secno** **stage1** **stage2** **traytype** *keyword=value*

Keywords:

NPASS TRAY-SPACE DIAM SYSFAC OVER-DESIGN EFF FLOOD-METH P-UPDATE DECK-THICK DC-OFC-WALL

Keywords for bubble cap trays:

CAP-DIAM NCAPS NROWS CAP-SPACE SKIRT-HT

Keywords for sieve trays:

HOLE-DIAM HOLE-AREA

Keywords for valve trays:

VALVE-TYPE VALVE-DEN NVALVES

Keywords for ballast trays:

VALVE-MAT VALVE-THICK

Keywords for float valve trays:

VALVE-LIFT DC-RTIME DC-EDGE

Optional keywords:

WEIR-HT-A WEIR-HT-B WEIR-HT-C WEIR-HT-D DC-CLEAR-SIDE DC-CLEAR-CTR DC-CLEAR-OFC DC-WTOP-SIDE DC-WTOP-CTR DC-WTOP-OFC DC-WBOT-SIDE DC-WBOT-CTR DC-WBOT-OFC DC-HT-SIDE DC-HT-CTR DC-HT-OFC

STR-TRAY-RA1 **stripid** **secno** *keyword=value*

Keywords:

MAX-FLOOD-F MAX-DCBUP-F

STR-PACK-SIZE **stripid** **secno** **stage1** **stage2** **packtype** *keyword=value*

Keywords:

PACK-MAT PACK-SIZE VENDOR PACK-FAC SPAREA VOIDFR STICH1 STICH2 STICH3 SYSFAC OVER-DESIGN PACK-HT HETP PACK-THICK CS-APP CS-FLOOD CS-DESIGN DPMAX-SEC DPMAX-PACK DPMETH P-UPDATE

STR-PACK-RATE **stripid** **secno** **stage1** **stage2** **packtype** *keyword=value*

Keywords:

PACK-MAT PACK-SIZE VENDOR PACK-FAC SPAREA VOIDFR STICH1 STICH2 STICH3 SYSFAC OVER-DESIGN PACK-HT HETP PACK-THICK DIAM CS-FLOOD DPMETH P-UPDATE

STR-PACK-RA1 **stripid** **secno** **MAX-FLOOD-F=value**

SUBROUTINE *keyword=value*

Keywords:

TRAYSR PACKSR

TRSR-VECS *keyword=value*

Keywords:

TRNINT TRNREAL

TRSR-INT VALUE-LIST=values
TRSR-REAL VALUE-LIST=values
PCKSR-VECS *keyword=value*

Keywords:

PCKNINT PCKNREAL

PCKSR-INT VALUE-LIST=values
PCKSR-REAL VALUE-LIST=values

Input Language Description

PARAM

Use to enter the number of stages and columns, and other parameters for RADFRAC, MULTIFRAC, and PETROFRAC. See Chapter 15 for keywords and keyword descriptions for the PARAM sentence.

P-UPDATE and P-FIX are used to invoke integrated pressure drop calculations. If you invoke these calculations, Aspen Plus uses the pressure drop computed from the hydraulic calculations to update the column pressure profile. The pressure specifications entered in the P-SPEC statement are used to initialize the pressure profile, and to fix the top or bottom pressure. Integrated pressure drop calculations are not allowed for tray sizing calculations.

P-UPDATE	**P-UPDATE=YES**	Pressure profile is to be updated from the computed pressure drop
	P-UPDATE=NO	Pressure profile is not to be updated from the computed pressure drop (Default)
P-FIX	**P-FIX=TOP**	Pressure at the top of column is kept constant during pressure updating (Default)
	P-FIX=BOTTOM	Pressure at the bottom of column is kept constant during pressure updating

CONVERGENCE

Use to enter flooding method for Koch Flexitray and Nutter Float Valve tray sizing and rating calculations and other TKWs for RadFrac, PetroFrac, and MultiFrac.

KOCH-CORR	**KOCH-CORR=B960**	Use curves in Bulletin 960 (KochEngineering Company, Inc.) for Koch Flexitray sizing/rating calculations. (Default)
	KOCH-CORR=B960-1	Use curves in Bulletin 960-1 (KochEngineering Company, Inc.) for Koch Flexitray sizing/rating calculations.
NUTTER-CORR.....	**NUTTER-CORR=ASPEN90**	Use ASPEN90 version of curve fitting for curves in Nutter Valve Tray Design Manual for Nutter Float Valve tray sizing/rating calculations.
	NUTTER-CORR=ASPEN96	Use ASPEN96 version of curve fitting for curves in Nutter Valve Tray Design Manual for Nutter Float Valve tray sizing/rating calculations.

TRAY-SIZE, STR-TRAY-SIZE

Use to enter specifications for tray sizing calculations. Column section diameter is determined from the specified number of passes, tray spacing, flooding approach, and other tray details. You can divide a column into any number of sections. Each section can have a different tray type and diameter. Tray details can vary from one section to another.

stripid ..... Stripper ID. Use for PETROFRAC only.

secno ..... Column section number. Must be sequential, starting with 1.

col ..... Column number. Use for MULTIFRAC only.

stage1 ..... Initial stage number of the section. If a condenser is present, *stage1* cannot be 1.

stage2 ..... Final stage number of the section. If a kettle reboiler is present, *stage2* cannot be NSTAGE.

traytype ..... Tray type:

CAPS	Bubble caps trays
SIEVE	Sieve trays
BALLAST	Glitsch ballast trays
FLEXI	Koch flexitrays
FLOAT	Nutter float valve trays

NPASS ..... Number of passes on each tray. Maximum of 4 passes are allowed. See Figures 16.1 through 16.4 for schematic diagrams.

NPASS=1	One-pass tray (Default)
NPASS=2	Two-pass tray
NPASS=3	Three-pass tray
NPASS=4	Four-pass tray

TRAY-SPACE ..... Tray spacing (Default=24 in. (609.6 mm))

FLOOD-FAC ..... Flooding approach, given as a fraction of flooding (Default=0.8)

SYSFAC ..... System foaming factor (Default=1.0). Suggested values are:

Ballast Trays

Service	SYSFAC
Non-foaming systems	1.00
Fluorine systems	0.90
Moderate foamers (such as oil absorbers, amine, and glycol regenerators)	0.85
Heavy foamers (such as amine and glycol absorbers)	0.73
Severe foamers (such as MEK units)	0.60
Foam stable systems (such as caustic regenerators)	0.30

Flexitrays

Service	SYSFAC
Depropanizers	0.85-0.95
Absorbers	0.85
Vacuum towers	0.85
Amine regenerators	0.85
Amine contactors	0.70-0.80
High pressure deethanizers	0.75-0.80
Glycol contactors	0.70-0.75

Float Valve Trays

Service	SYSFAC
Non-foaming	1.00
Low-foaming	0.90
Moderate-foaming	0.75
High-foaming	0.60

SLOT-AREA ..... Slot area, given as a fraction of the active area. Use only when *traytype* is CAPS and FLOOD-METH=FAIR or USER. (Default=0.12)

HOLE-AREA ..... Hole area, given as a fraction of the active area. Use only when *traytype* is SIEVE and FLOOD-METH=FAIR or USER. (Default=0.12)

MIN-DIAM..... Minimum column diameter (Default=12 in. (304.8 mm))

MIN-DCAREA..... Minimum downcomer area, given as a fraction of the total tray cross-sectional area (Default=0.1)

OVER-DESIGN ..... Over-design factor, a multiplier for the column loading to reflect the expected maximum or minimum loading for the column. OVER-DESIGN cannot be used if P-UPDATE=YES. (Default=1.0)

FLOOD-METH ..... Flooding calculation method. When *traytype* is CAPS, SIEVE, or BALLAST, use FAIR, GLITSCH, or USER method. The FAIR method provides a more conservative estimate for flooding approach. When traytype is FLEXI, use B960 or B960-1. B960-1 is recommended.

FLOOD-METH=FAIR	Fair method
FLOOD-METH=GLITSCH	Glitsch method. Designed for ballast trays. De-rates the results by 15% for bubble caps and 5% for sieve trays. (Default)
FLOOD-METH=USER	User-supplied method
FLOOD-METH=B960	Use curves in Bulletin 960 (KochEngineering Company, Inc.) for Koch Flexitray sizing/rating calculations.
FLOOD-METH=B960-1	Use curves in Bulletin 960-1 (KochEngineering Company, Inc.) for Koch Flexitray sizing/rating calculations.

TRAY-RATE, STR-TRAY-RATE

Use to enter column diameter and other tray details for tray rating calculations. Tray performance parameters, such as flooding approach, downcomer backup, and pressure drop are calculated. You can turn off the pressure updating calculations for a section locally. You can also divide a column into any number of sections. Each section can have a different tray type and diameter. Tray details can vary from one section to another.

stripid ..... Stripper ID. Use for PETROFRAC only.

secno ..... Column section number. Must be sequential, starting with 1.

col..... Column number. Use for MULTIFRAC only.

stage1..... Initial stage number of the section. If a condenser is present, *stage1* cannot be 1.

stage2..... Final stage number of the section. If a kettle reboiler is present, *stage2* cannot be NSTAGE.

traytype ..... Tray type:

CAPS	Bubble caps trays
SIEVE	Sieve trays
BALLAST	Glitsch ballast trays

	FLEXI	Koch flexitrays
	FLOAT	Nutter float valve trays

NPASS..... Number of passes on each tray. Maximum of four is allowed. See Figures 16.1 through 16.4 for schematic diagrams.

NPASS=1	One-pass tray (Default)
NPASS=2.	Two-pass tray
NPASS=3	Three-pass tray
NPASS=4	Four-pass tray

TRAY-SPACE ..... Tray spacing (Default=24 in. (609.6 mm))

DIAM ..... Column section diameter

SYSFAC..... System foaming factor (Default=1.0). Suggested values are:

Ballast Trays

Service	SYSFAC
Non-foaming systems	1.00
Fluorine systems	0.90
Moderate foamers (such as oil absorbers,amine, and glycol regenerators)	0.85
Heavy foamers (such as amine and glycol absorbers)	0.73
Severe foamers (such as MEK units)	0.60
Foam stable systems (such as caustic regenerators)	0.30

Flexitrays

Service	SYSFAC
Depropanizers	0.85-0.95
Absorbers	0.85
Vacuum towers	0.85
Amine regenerators	0.85
Amine contactors	0.70-0.80
High pressure deethanizers	0.75-0.80
Glycol contactors	0.70-0.75

Float Valve Trays

Service	SYSFAC
Non-foaming	1.00
Low-foaming	0.90
Moderate-foaming	0.75
High-foaming	0.60

OVER-DESIGN..... Over-design factor. A multiplier for the column loading to reflect the expected maximum or minimum loading for the column. You cannot use OVER-DESIGN if P-UPDATE=YES. (Default=1.0)

EFF..... Overall efficiency. Defined as the ratio of number of theoretical stages to number of actual trays. Do not enter EFF if you specified STAGE-EFF, L1-STAGE-EFF, L2-STAGE-EFF, COMP-EFF, L1-COMP-EFF, L2-COMP-EFF, STR-STAGE-EFF or STR-COMP-EFF. (See Chapter 15.) (Default=1.0)

FLOOD-METH ..... Flooding calculation method. When *traytype* is CAPS, SIEVE, or BALLAST, use FAIR, GLITSCH, GLITSCH6, or USER method. The FAIR method provides a more conservative estimate for flooding approach. When traytype is FLEXI, use B960 or B960-1. When VALVE-TYPE is S, AO, or TO, B960 must be used. Otherwise, B960-1 is recommended.

FLOOD-METH=FAIR	Fair method
FLOOD-METH=GLITSCH	Glitsch method. Designed for ballast trays. De-rates the results by 15% for bubble caps and 5% for sieve trays. (Default)
FLOOD-METH=GLITSCH6	Glitsch method from Bulletin 4900, Edition 6.
FLOOD-METH=USER	User-supplied method
FLOOD-METH=B960	Use curves in Bulletin 960 (KochEngineering Company, Inc.) for Koch Flexitray sizing/rating calculations.
FLOOD-METH=B960-1	Use curves in Bulletin 960-1 (KochEngineering Company, Inc.) for Koch Flexitray sizing/rating calculations.

P-UPDATE .....

P-UPDATE=YES	Updates pressure profile for the section. You must also specify P-UPDATE=YES in the PARAM sentence.
P-UPDATE=NO	Does not update pressure profile for the section (Default)

DECK-THICK ..... Tray deck thickness. Use when *traytype* is SIEVE, BALLAST, and FLOAT. Valid entries for deck thickness are:

Gauge	Inches	Millimeters
3	0.250	6.35
10	0.134	3.40 (Default)
12	0.104	2.64
14	0.074	1.88

Do not enter the values in gauge. They are listed here for reference only.

DC-OFC-WALL ..... Distance between column wall and off-center downcomer (on side near wall). For three-pass and four-pass trays.

CAP-DIAM ..... Cap diameter. Use when *traytype* is CAPS only. Valid entries for cap diameter are:

Inches	Millimeters
3	76.2 (Default)
4	101.6
6	152.4

The cap diameter is used to retrieve cap characteristics based on the standard cap designs. Table 16.2 gives standard cap designs for the three cap sizes. The default for cap diameter depends on the column diameter as follows:

For Column Diameter ≤ 48 in. (1219.2 mm),
Default is CAP-DIAM=3 in. (76.2 mm)

For Column Diameter > 48 in. (1219.2 mm),
Default is CAP-DIAM=4 in. (101.6 mm)

NCAPS..... Number of caps per panel. Use when *traytype* is CAPS only. The first entry is for panel A, the second for panel B, the third for panel C, and the fourth for panel D. Enter an asterisk for an entry that has a missing value. The number of entries depends on the number of flow passes:

For	Enter
One-pass tray	A single value for panel A
Two-pass tray	Up to two values, one for panel A and one for panel B
Three-pass tray	Up to three values, one for each of the three panels (A, B, and C)
Four-pass tray	Up to four values, one for each of the four panels (A, B, C, and D)

The value for NCAPS applies for each panel. For two-pass trays, there are two A panels for tray AA, and two B panels for tray BB. Therefore, the number of caps per panel is the number of caps per tray divided by two for two-pass trays. Similar consideration is necessary when you enter NCAPS for three- and four-pass trays.

If you enter only one value for multi-pass trays, that value applies to all panels. If you do not supply NCAPS, it is estimated from CAP-SPACE.

NROWS..... Number of rows per panel. Use when *traytype* is CAPS only. The first entry is for panel A, the second for panel B, the third for panel C, and the fourth for panel D. Enter an asterisk for an entry that has a missing value. The number of entries depends on the number of flow passes:

For	Enter
One-pass tray	A single value for panel A
Two-pass tray	Up to two values, one for panel A and one for panel B
Three-pass tray	Up to three values, one for each of the three panels (A, B, and C)
Four-pass tray	Up to four values, one for each of the four panels (A, B, C, and D)

The value for NROWS applies for each panel. For two-pass trays, there are two A panels for tray AA, and two B panels for tray BB. Therefore, the number of caps per panel is the number of caps per tray divided by two for two-pass trays. Similar consideration is necessary when you enter NROWS for three- and four-pass trays.

If you enter only one value for multi-pass trays, that value applies to all panels. If you do not supply NROWS, it is estimated from CAP-SPACE.

CAP-SPACE..... Cap spacing measured between the outside diameter of adjacent caps. Use when *traytype* is CAPS only. You cannot use CAP-SPACE if you specified NCAPS and NROWS. (Default=25% of cap diameter)

SKIRT-HT..... Skirt height. Use when *traytype* is CAPS only. Valid skirt heights are:

Inches	Millimeters
0.5	12.7
1.0	25.4 (Default)
1.5	38.1

HOLE-DIAM ..... Sieve hole diameter. Use when *traytype* is SIEVE only. (Default=0.5 in. (12.7 mm))

HOLE-AREA ..... Sieve hole area given as a fraction of the active area. Use when *traytype* is SIEVE only. (Default=0.12)

VALVE-TYPE ..... Valve type. Use when *traytype* is BALLAST, FLEXI, or FLOAT. Valid valve types are:

Tray Type	VALVE-TYPE	Default
BALLAST	V-1, V-4	V-1
FLEXI	A-14, A-16, T-14, T-16, A-18, T-18, K-8, S, AO, TO	A-14
FLOAT	BDP, BDH	BDP

VALVE-DEN ..... Valve density, defined as the number of valves per unit active area. Use when *traytype* is BALLAST, FLEXI or FLOAT. You cannot use VALVE-DEN if you specified NVALVES. See Table 16.1 for unit options. (Default=13/SQFT (139.92/SQM))

NVALVES ..... Number of valves per panel. Use when *traytype* is BALLAST, FLEXI, or FLOAT. The first entry is for panel A, the second for panel B, the third for panel C, and the fourth for panel D. You cannot use NVALVES if you specified VALVE-DEN. Enter an asterisk for an entry that has a missing value. The number of entries depends on the number of flow passes:

For	Enter
One-pass tray	A single value for panel A
Two-pass tray	Up to two values, one for panel A and one for panel B
Three-pass tray	Up to three values, one for each of the three panels (A, B, and C)
Four-pass tray	Up to four values, one for each of the four panels (A, B, C, and D)

The value for NVALVES applies for each panel. For two-pass trays, there are two A panels for tray AA, and two B panels for tray BB. Therefore, the number of caps per panel is the number of caps per tray divided by two for two-pass trays. Similar consideration is necessary when you enter NVALVES for three- and four-pass trays.

If you enter only one value for multi-pass trays, that value applies to all panels. If you do not supply NVALVES, it is estimated from VALVE-DEN.

VALVE-MAT ..... Valve material. Use when *traytype* is BALLAST only.

VALVE-MAT=CS	Carbon steel (Default)
VALVE-MAT=SS	Stainless steel
VALVE-MAT=NI	Nickel
VALVE-MAT=LEAD	Lead
VALVE-MAT=TI	Titanium
VALVE-MAT=MONEL	Monel
VALVE-MAT=HASTELLOY	Hastelloy
VALVE-MAT=ALUMINUM	Aluminum
VALVE-MAT=COPPER	Copper

VALVE-THICK..... Valve thickness. Use when *traytype* is BALLAST only. Valid valve thicknesses are:

Gauge	Inches	Millimeters
10	0.134	3.40
12	0.104	2.64
14	0.074	1.88
16	0.060	1.52 (Default)
18	0.050	1.27
20	0.037	0.94

Do not enter the values in gauge. They are listed here for reference only.

VALVE-LIFT..... Valve lift. Use when *traytype* is FLOAT only. Valid valve lift entries are:

Inches	Millimeters
0.313	7.95 (Default)
0.375	9.53
0.438	11.13
0.500	12.70

DC-RTIME ..... Downcomer residence time. Use when *traytype* is FLOAT only. (Default=4 seconds)

DC-EDGE ..... Downcomer edge type. Use when *traytype* is FLOAT only.

DC-EDGE=SHARP	Sharp downcomer edge (Default)
DC-EDGE=RADIUS	Radius downcomer edge

WEIR-HT-A, WEIR-HT-B, WEIR-HT-C, WEIR-HT-D Outlet weir height for panel A, panel B, panel C, and panel D, respectively. The number of entries depends on the number of flow passes.

For	Enter
One-pass tray	A single value for panel A
Two-pass tray	Up to two values, one for panel A and one for panel B
Three-pass tray	Up to three values, one for each of the three panels (A, B, and C)
Four-pass tray	Up to four values, one for each of the four panels (A, B, C, and D)

The panel A value defaults to 2 in. (50.8 mm) for valve and sieve trays. The panel A default for bubble cap trays is a function of cap diameter so as to provide adequate dynamic seal and minimum skirt clearance. The defaults are:

Cap diameter		Default weir height	
Inches	**Millimeters**	**Inches**	**Millimeters**
3	76.2	2.75	69.85
4	101.6	3.00	76.20
6	152.4	3.25	82.55

DC-CLEAR-SIDE, DC-CLEAR-CTR, DC-CLEAR-OFC ..... Downcomer clearance for side downcomer, center downcomer, and off-center downcomer, respectively. The number of entries depends on the number of flow passes.

For	Enter
One-pass tray	A single value for the side downcomer
Two-pass tray	Up to two values, one for the side downcomer and one for the center downcomer
Three-pass tray	Up to two values, one for the side downcomer and one for the off-center downcomer
Four-pass tray	Up to three values, one for the side downcomer, one for the center downcomer and one for the off-center downcomer

Values for center and off-center downcomers default to the value for the side downcomer. The default for side downcomer is calculated by subtracting 0.5 in. (12.7 mm) from the specified value of WEIR-HT, to provide the minimum downcomer seal.

DC-WTOP-SIDE, DC-WTOP-CTR, DC-WTOP-OFC ..... Top downcomer width for side downcomer, center downcomer, and off-center downcomer, respectively. The number of entries depends on the number of flow passes:

For	Enter
One-pass tray	A single value for the side downcomer
Two-pass tray	Up to two values, one for the side downcomer and one for the center downcomer
Three-pass tray	Up to two values, one for the side downcomer and one for the off-center downcomer
Four-pass tray	Up to three values, one for the side downcomer, one for the center downcomer and one for the off-center downcomer

If you do not specify the top downcomer widths, they are estimated from the downcomer area as follows:

NPASS	Downcomer area/tray cross-sectional area
1	0.10
2	0.12
3	0.15
4	0.20

DC-WBOT-SIDE, DC-WBOT-CTR, DC-WBOT-OFC ..... Bottom downcomer width for side downcomer, center downcomer, and off-center downcomer, respectively. The number of entries depends on the number of flow passes:

For	Enter
One-pass tray	A single value for the side downcomer
Two-pass tray	Up to two values, one for the side downcomer and one for the center downcomer
Three-pass tray	Up to two values, one for the side downcomer and one for the off-center downcomer
Four-pass tray	Up to three values, one for the side downcomer, one for the center downcomer and one for the off-center downcomer

If you do not specify the bottom downcomer widths, the default assumes a straight downcomer (same width at bottom as at top).

DC-HT-SIDE, DC-HT-CTR, DC-HT-OFC ..... Straight height above slope in downcomer, for side downcomer, center downcomer, and off-center downcomer, respectively. Use for sloped downcomer only. The number of entries depends on the number of flow passes:

For	Enter
One-pass tray	A single value for the side downcomer
Two-pass tray	Up to two values, one for the side downcomer and one for the center downcomer
Three-pass tray	Up to two values, one for the side downcomer and one for the off-center downcomer
Four-pass tray	Up to three values, one for the side downcomer, one for the center downcomer and one for the off-center downcomer

(Default=0)

TRAY-RATE1, STR-TRAY-RA1

Use to enter additional tray rating specifications to be used for column targeting hydraulic analysis calculations. Specify when the HYDANAL report option is chosen in the REPORT sentence for RADFRAC, MULTIFRAC, or PETROFRAC.

stripid ..... Stripper ID. Use for PETROFRAC only.

secno ..... Column section number. Must correspond to a section number specified in TRAY-RATE or STR-TRAY-RATE sentence.

MAX-FLOOD-F ..... Vapor flooding approach to maximum (Default=0.85)

MAX-DCBUP-F ..... Liquid flooding approach to maximum due to downcomer backup (Default=0.5)

PACK-SIZE, STR-PACK-SIZE

Use to enter specifications for packing sizing calculations. Column section diameter is determined from fractional approach to maximum capacity or design capacity factor. Optionally, you can impose the maximum pressure drop (per unit height or for the section) as an additional constraint for the diameter calculations. In addition, you can turn off the pressure updating calculations for the section locally. You can divide the column into any number of sections. Each section can have a different packing type and diameter. Packing specifications can vary from one section to another. See Tables 16.3 through 16.7 for entering built-in packing types.

stripid ..... Stripper ID. Use for PETROFRAC only.

secno ..... Column section number. Must be sequential, starting with 1.

col ..... Column number. Use for MULTIFRAC only.

stage1 ..... Initial stage number of the section. If a condenser is present, *stage1* cannot be 1.

stage2 ..... Final stage number of the section. If a kettle reboiler is present, *stage2* cannot be NSTAGE.

packtype ..... Packing type. Use to determine the proper calculation procedure and to retrieve packing characteristics for random and structural packings from the databank. See Tables 16.3 through 16.8 for the available packing types.

PACK-MAT ..... Packing material. Use to retrieve the packing characteristics from the databank. For random packings, it is not necessary to enter PACK-MAT if you specified PACK-FAC. See Tables 16.3 through 16.8 for valid materials of different packing types.

PACK-MAT=CARBON	Carbon
PACK-MAT=CERAMIC	Ceramic
PACK-MAT=METAL	Metal

	PACK-MAT=METAL-32	1/32 in. metal
	PACK-MAT=METAL-16	1/16 in. metal
	PACK-MAT=PLASTIC	Plastic
	PACK-MAT=STEEL	Steel
	PACK-MAT=POLYPROP	Polypropylene
	PACK-MAT=STANDARD	Standard
PACK-SIZE	Packing size. Use to retrieve the packing characteristics from the databank. For random packings, it is not necessary to enter PACK-SIZE if you specified PACK-FAC. See Tables 16.3 through 16.8 for valid sizes of different packing types and materials.	
VENDOR	Packing vendor. Use to retrieve the packing characteristics and select the calculation method.	
	VENDOR=MTL	MTL packing
	VENDOR=NORTON	Norton packing
	VENDOR=GENERIC	Generic packing
	VENDOR=SULZER	Sulzer packing
	VENDOR=KOCH	Koch packing
	VENDOR=RASCHIG	Raschig Packing
PACK-FAC	Packing factor. Use for random packings (except IMTP) only. Use to override the value from the databank. If you specify PACK-FAC, you do not need to specify PACK-MAT and PACK-SIZE. See Table 16.1 for unit options.	
SPAREA	Specific surface area of the packing. Use to override the value from the databank. This is a required parameter for the Stichlmair model.[1]	
VOIDFR	Void fraction of the packing. Use to override the value from the databank. This is a required parameter for the Stichlmair model.[1]	
STICH1, STICH2, STICH3	Stichlmair model parameters. Use to override values from the databank.[1]	
SYSFAC	System foaming factor (Default=1.0)	
OVER-DESIGN	Over-design factor, a multiplier for the column loading to reflect the expected maximum or minimum loading for the column. You cannot use OVER-DESIGN if P-UPDATE=YES. (Default=1.0)	
PACK-HT	Packed height. Use to determine the HETP for the section. You cannot use PACK-HT, if you specified HETP.	
HETP	Height Equivalent of a Theoretical Plate (HETP) for the section. HETP=packed height/number of stages. You cannot use HETP, if you specified PACK-HT.	
PACK-THICK	Sheet thickness for Sulzer structured packing	
CS-APP	Fractional approach to maximum capacity. Use to determine the column section diameter. (Default=1.0 for Raschig packings; 0.62 for other packings)	

1 *The Stichlmair model is used for calculating liquid holdup of both random and structured packings. It is also used to calculate pressure drop and capacity if DPMETH=STICHL.*

CS-FLOOD ..... Capacity factor at flooding. Can be used to override internally calculated value. The capacity factor is defined as follows:

$$CS - FLOOD = \upsilon_s \sqrt{\frac{\rho_v}{\rho_L - \rho_v}}$$

Where:
υ_S = Superficial velocity of vapor to the packing
ρ_V = Density of vapor to the packing
ρ_L = Density of liquid from the packing

CS-DESIGN ..... Design capacity factor. Use to determine the column section diameter instead CS-APP. You cannot use CS-DESIGN if you specified CS-APP.

DPMAX-SEC..... Maximum pressure drop for the section. Can be used as an additional constraint in the diameter calculations. You cannot use DPMAX-SEC if you specified DPMAX-PACK. The unit keyword for DPMAX-SEC is PDROP. See Table 16.7 for unit options.

DPMAX-PACK ..... Maximum pressure drop per unit height. Can be used as an additional constraint in the diameter calculations. You cannot use DPMAX-PACK if you specified DPMAX-SEC. The units keyword for DPMAX-PACK is PDROP-PER-HT. See Table 16.7 for unit options.

DPMETH ..... Pressure drop calculation method. You can use DPMETH for random packings if you specified VENDOR=GENERIC.

DPMETH=ECKERT	Eckert method (Default)
DPMETH=NORTON	Norton method
DPMETH=PRAHL	Prahl method
DPMETH=TSAI	Tsai method
DPMETH=STICHL	Stichlmair model
DPMETH=USER	User-supplied method

P-UPDATE .....

P-UPDATE=YES	Pressure profile is updated for the section. You must also specify P-UPDATE=YES in the PARAM sentence.
P-UPDATE=NO	Pressure profile is not updated for the section (Default)

PACK-RATE, STR-PACK-RATE

Use to enter specifications for rating calculations for packing. You must specify column section diameter. Fractional approach to maximum capacity and pressure drop are calculated. In addition, you can turn off the pressure updating calculations for a section locally. You can divide the column into any number of sections. Each section can have a different packing type and diameter. Packing specifications can vary from one section to another. See Tables 16.3 through 16.7 for built-in packing types.

stripid ..... Stripper ID. Use for PETROFRAC only.

secno ..... Column section number. Must be sequential, starting with 1.

col..... Column number. Use for MULTIFRAC only.

stage1..... Starting stage number of the section. If a condenser is present, *stage1* cannot be 1.

stage2..... Ending stage number of the section. If a kettle reboiler is present, *stage2* cannot be NSTAGE.

packtype ..... Packing type. Use to determine the proper calculation procedure and to retrieve packing characteristics for random and structural packings from the databank. See Tables 16.3 through 16.8 for details on the available packing types.

PACK-MAT ..... Packing material. Use to retrieve the packing characteristics from the databank. For random packings, it is not necessary to enter PACK-MAT if you specified PACK-FAC. See Tables 16.3 through 16.8 for valid materials of different packing types.

PACK-MAT=CARBON	Carbon
PACK-MAT=CERAMIC	Ceramic
PACK-MAT=METAL	Metal
PACK-MAT=METAL-32	1/32 in. metal
PACK-MAT=METAL-16	1/16 in. metal
PACK-MAT=PLASTIC	Plastic
PACK-MAT=STEEL	Steel
PACK-MAT=POLYPROP	Polypropylene
PACK-MAT=STANDARD	Standard

PACK-SIZE ..... Packing size. Use to retrieve the packing characteristics from the databank. For random packings, it is not necessary to enter PACK-SIZE if you specified PACK-FAC. See Tables 16.3 through 16.8 for valid sizes of different packing types and materials.

VENDOR ..... Packing vendor. Use to retrieve the packing characteristics and select the calculation method.

VENDOR=MTL	MTL packing
VENDOR=NORTON	Norton packing
VENDOR=GENERIC	Generic packing
VENDOR=SULZER	Sulzer packing
VENDOR=KOCH	Koch packing
VENDOR=RASCHIG	Raschig Packing

PACK-FAC ..... Packing factor. Use for random packings (except IMTP) only. Use to override the value from the databank. If you specified PACK-FAC, you do not need to enter PACK-MAT and PACK-SIZE.

SPAREA ..... Specific surface area of the packing. Use to override the value from the databank. This is a required parameter for the Stichlmair model.[2]

VOIDFR ..... Void fraction of the packing. Use to override the value from the databank. This is a required parameter for the Stichlmair model.[2]

STICH1, STICH2, STICH3 ..... Stichlmair model parameters. Use to override values from the databank.[2]

SYSFAC ..... System foaming factor (Default=1.0)

OVER-DESIGN ..... Over-design factor. A multiplier for the column loading to reflect the expected maximum or minimum loading for the column. You cannot use OVER-DESIGN if P-UPDATE=YES. (Default=1.0)

PACK-HT ..... Packed height. Use to determine the HETP for the section. You cannot use PACK-HT if you specified HETP.

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2 The Stichlmair model is used for calculating liquid holdup of both random and structured packings. It is also used to calculate pressure drop and capacity if DPMETH=STICHL.

HETP ..... Height Equivalent of a Theoretical Plate (HETP) for the section. HETP=packed height/number of stages. You cannot use HETP if you specified PACK-HT.

PACK-THICK..... Sheet thickness for Sulzer structured packing

DIAM ..... Column section diameter

CS-FLOOD ..... Capacity factor at flooding. Can be used to override internally calculated value. The capacity factor is defined as follows:

$$CS - FLOOD = \upsilon_s \sqrt{\frac{\rho_v}{\rho_L - \rho_v}}$$

Where:
υ_S = Superficial velocity of vapor to the packing
ρ_V = Density of vapor to the packing
ρ_L = Density of liquid from the packing

DPMETH ..... Pressure drop calculation method. You can use DPMETH for random packings if you specify VENDOR=GENERIC.

DPMETH=ECKERT	Eckert method (Default)
DPMETH=NORTON	Norton method
DPMETH=PRAHL	Prahl method
DPMETH=TSAI	Tsai method
DPMETH=STICHL	Stichlmair model
DPMETH=USER	User-supplied method

P-UPDATE .....

P-UPDATE=YES	Pressure profile is updated for the section. You must also specify P-UPDATE=YES in the PARAM sentence.
P-UPDATE=NO	Pressure profile is not updated for the section (Default)

THETA..... Corrugation angle of structured packing, in degrees. Only used for rate-based calculations in RADFRAC. (Default = retrieved from an internal database based on the packing type, vendor, material, and dimension, or 45 degrees if no value is available in the database.)

PACK-RATE1, STR-PACK-RA1

Use to enter additional packing rating specifications to be used for column targeting hydraulic analysis calculations. Specify when the HYDANAL report option is chosen in the REPORT sentence for RADFRAC, MULTIFRAC, or PETROFRAC.

stripid ..... Stripper ID. Use for PETROFRAC only.

secno ..... Column section number. Must correspond to a section number specified in PACK-RATE or STR-PACK-RATE sentence.

MAX-FLOOD-F ..... Vapor flooding approach to maximum (Default=0.85)

SUBROUTINE

Use to specify user-supplied subroutine names for tray/packing sizing and rating calculations. To invoke the user tray sizing and rating subroutine for calculations in a section, you must also specify FLOOD-METH=USER in a TRAY-SIZE, STR-TRAY-SIZE, TRAY-RATE, or STR-TRAY-RATE sentence. To invoke the user packing sizing and rating subroutine for calculations in a section, you must also specify DP-METH=USER in a PACK-SIZE, STR-PACK-SIZE, PACK-RATE, or STR-PACK-RATE sentence. For details on writing the user-supplied subroutine, see *Aspen Plus User Models*, Chapter 21.

TRAYSR..... User-supplied FORTRAN subroutine name for tray sizing and rating calculations

PACKSR..... User-supplied FORTRAN subroutine name for packing sizing and rating calculations

TRSR-VECS Use to define length of arrays for the user-supplied tray sizing and rating subroutine.

TRNINT..... Length of integer parameter array

TRNREAL..... Length of real parameter array

TRSR-INT Use to enter values for the integer parameter array of the user-supplied tray sizing subroutine.

VALUE-LIST ..... List of integer values

TRSR-REAL Use to enter values for the real parameter array of the user-supplied tray sizing subroutine.

VALUE-LIST ..... List of real values

PCKSR-VECS Use to define length of arrays for the user-supplied packing sizing and rating subroutine.

PCKNINT..... Length of integer parameter array

PCKNREAL..... Length of real parameter array

PCKSR-INT Use to enter values for the integer parameter array of the user-supplied packing sizing and rating subroutine.

VALUE-LIST ..... List of integer values

PCKSR-REAL Use to enter values for the real parameter array of the user-supplied packing sizing and rating subroutine.

VALUE-LIST ..... List of real values

Figure 16.1 Schematic Diagram of a One-Pass Tray

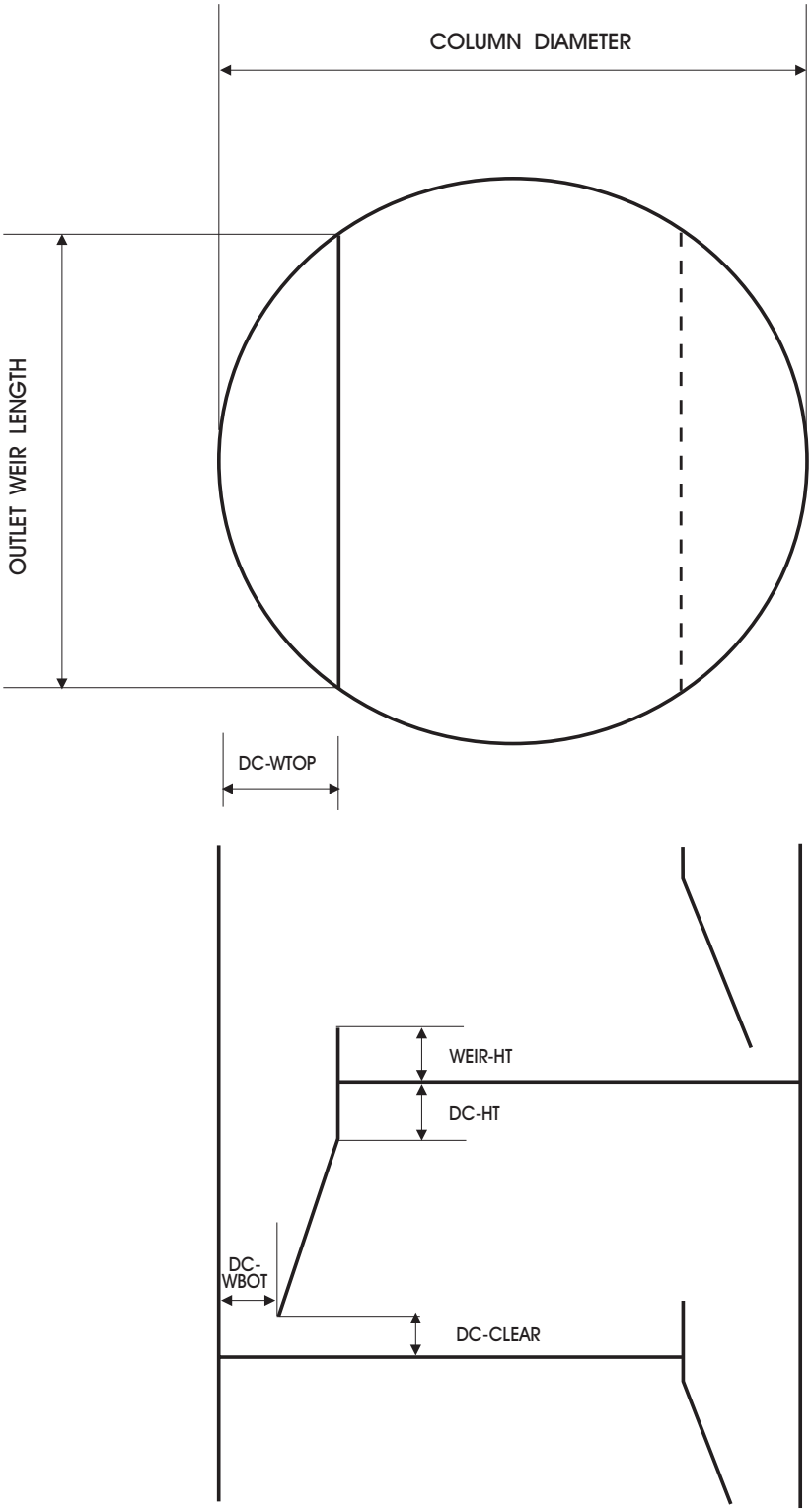


Figure 16.2 Schematic Diagram of a Two-Pass Tray

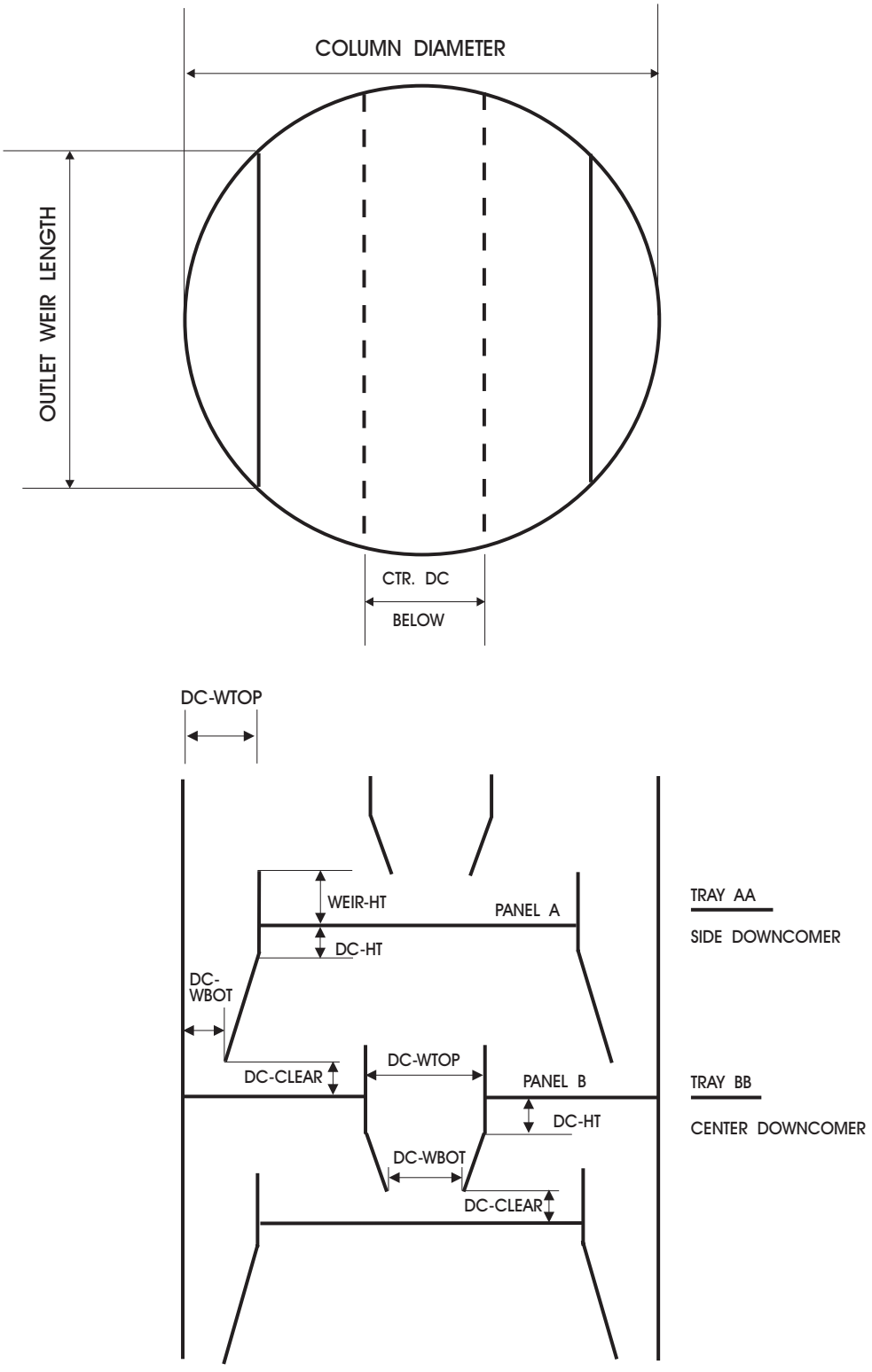


Figure 16.3 Schematic Diagram of a Three-Pass Tray

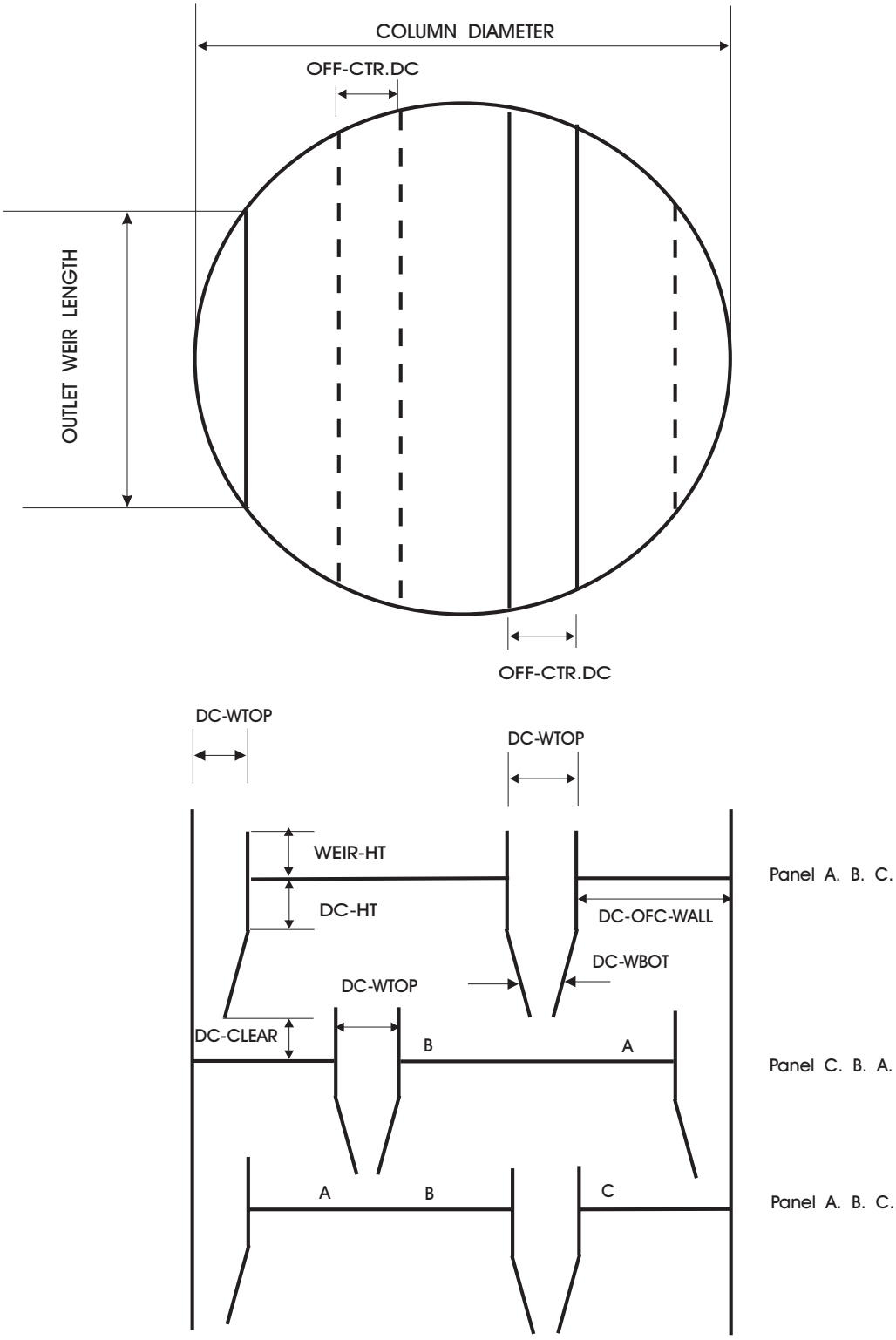
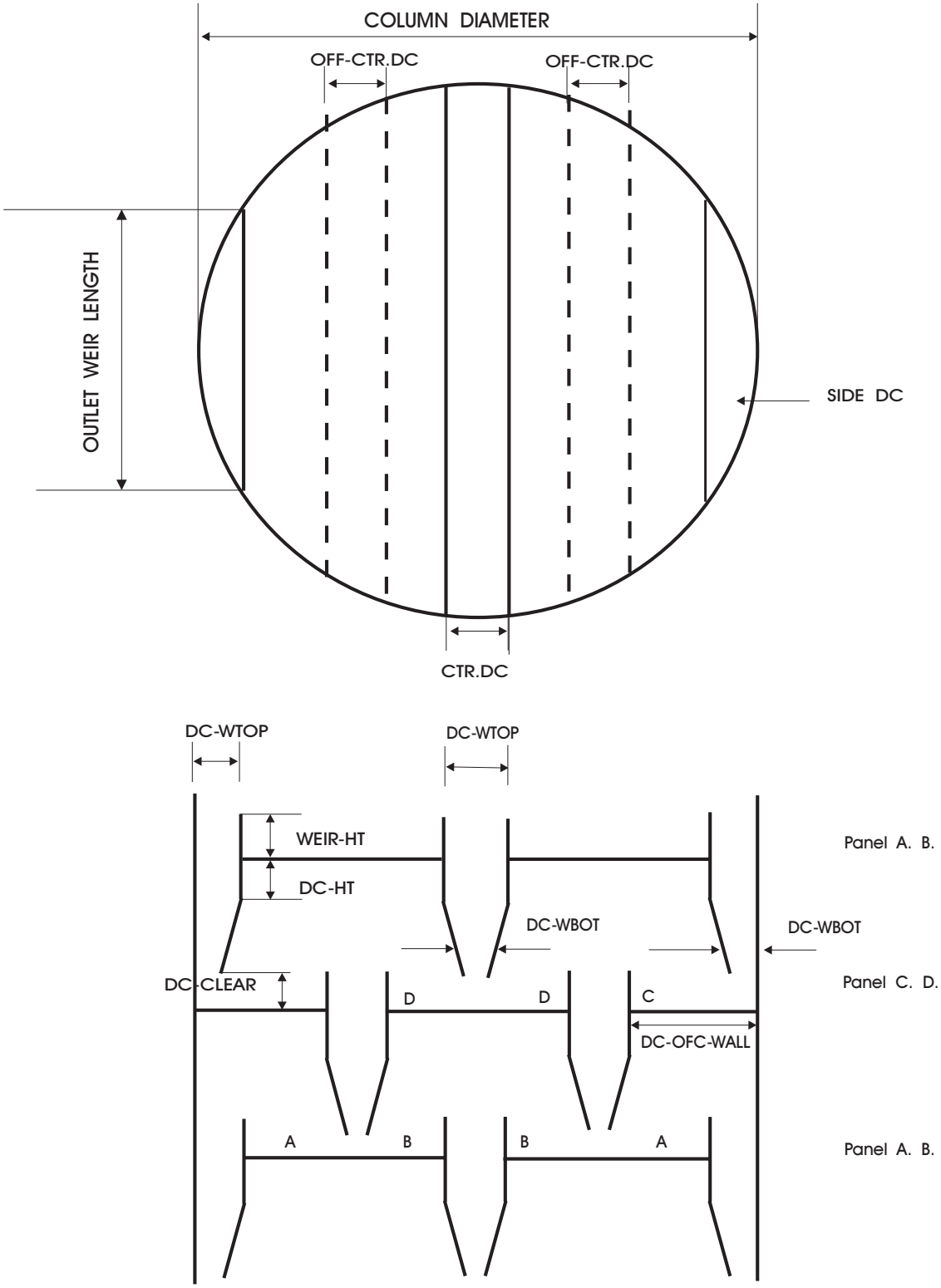


Figure 16.4 Schematic Diagram of a Four-Pass Tray



Accessing Variables in RADFRAC

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	Element
TRAY-SIZE	STAGE1, STAGE2, NPASS, TRAY-SPACE, FLOOD-FAC, SYSFAC, SLOT-AREA, HOLE-AREA, MIN-DIAM, MIN-DCAREA, OVER-DESIGN	secno	—
TRAY-RATE	STAGE1, STAGE2, NPASS, TRAY-SPACE, DIAM, SYSFAC, OVER-DESIGN, EFF, DECK-THICK, WEIR-HT-A, WEIR-HT-B, WEIR-HT-C, WEIR-HT-D, DC-CLEAR-SIDE, DC-CLEAR-CTR, DC-CLEAR-OFC, DC-WTOP-SIDE, DC-WTOP-CTR, DC-WTOP-OFC, DC-WBOT-SIDE, DC-WBOT-CTR, DC-WOT-OFC, DC-HT-SIDE, DC-HT-CTR, DC-HT-OFC, DC-OFC-WALL, CAP-DIAM, CAP-SPACE, SKIRT-HT, HOLE-DIAM, HOLE-AREA, VALVE-DEN, VALVE-THICK, VALVE-LIFT, DC-RTIME	secno	—
TRAY-RATE	NCAPS, NROWS, NVALVES	secno	†
PACK-SIZE	STAGE1, STAGE2, PACK-FAC, SPAREA, VOIDFR, STICH1, STICH2, STICH3, SYSFAC, OVER-DESIGN, PACK-HT, HETP, PACK-THICK, CS-APP, CS-FLOOD, CS-DESIGN, DPMAX-SEC, DPMAX-PACK	secno	—
PACK-RATE	STAGE1, STAGE2, PACK-FAC, SPAREA, VOIDFR, STICH1, STICH2, STICH3, SYSFAC, OVER-DESIGN, PACK-HT, HETP, DIAM, PACK-THICK, CS-FLOOD	secno	—

† Position in which you enter the variable. For variables in panels A through D, enter 1 through 4 for the elements.

Block Results

Hydraulic parameters:

Description	Sentence	Variable†	ID1	ID2
Liquid mass flow from stage	HYDRAULIC	L-MASSFLOW	stage	—
Vapor mass flow to stage	HYDRAULIC	V-MASSFLOW	stage	—
Liquid volume flow from stage	HYDRAULIC	L-VOLFLOW	stage	—
Vapor volume flow to stage	HYDRAULIC	V-VOLFLOW	stage	—
Density of liquid from stage	HYDRAULIC	RHOL	stage	—
Density of vapor to stage	HYDRAULIC	RHOV	stage	—
Viscosity of liquid from stage	HYDRAULIC	MUL	stage	—
Viscosity of vapor to stage	HYDRAULIC	MUV	stage	—
Surface tension of liquid from stage	HYDRAULIC	SIGMA	stage	—
Flow parameter	HYDRAULIC	FLOWPA	stage	—
Reduced vapor throughput	HYDRAULIC	QR	stage	—

† You can also access all block result variables for RADFRAC using the VECTOR-DEF sentence. See Chapter 29.

continued

Hydraulic parameters (continued)

Description	Sentence	Variable†	ID1	ID2
Liquid molecular weight	HYDRAULIC	MWL	stage	—
Vapor molecular weight	HYDRAULIC	MWV	stage	—
Marangoni index ††	HYDRAULIC	FMIDX	stage	—
Reduced F factor	HYDRAULIC	FFACR	stage	—

Tray sizing results:

Description	Sentence	Variable†	ID1	ID2
Maximum column section diameter	TSIZE-RESULT	DIAM	secno	—

Tray rating results:

Description	Sentence	Variable†	ID1	ID2
Maximum flooding factor	TRATE-RESULT	FLOOD-FAC	secno	—
Stage with maximum flooding factor	TRATE-RESULT	FLOOD-MAX	secno	—
Maximum downcomer backup	TRATE-RESULT	DCBA	secno	—
Maximum DC backup/tray spacing	TRATE-RESULT	DC-FLOOD	secno	—
Stage with maximum DC backup	TRATE-RESULT	DCBA-MAX	secno	—
Maximum downcomer velocity	TRATE-RESULT	DCV	secno	—
Stage with maximum DC velocity	TRATE-RESULT	DCV-MAX	secno	—
Section pressure drop	TRATE-RESULT	DPSEC	secno	—

Tray rating results for panel A:

Description	Sentence	Variable†	ID1	ID2
Stage flooding factor	TRATE-PANELA	FLOOD-FAC	stage	secno
Stage DC backup	TRATE-PANELA	DCBA	stage	secno
Stage DC backup/tray spacing	TRATE-PANELA	DC-FLOOD	stage	secno
Stage DC velocity	TRATE-PANELA	DCV	stage	secno
Stage DC velocity/design velocity†††	TRATE-PANELA	DCV-FLOOD	stage	secno
Stage pressure drop	TRATE-PANELA	DP	stage	secno

Tray rating results for panel B:

Description	Sentence	Variable†	ID1	ID2
Stage flooding factor	TRATE-PANELB	FLOOD-FAC	stage	secno
Stage DC backup	TRATE-PANELB	DCBA	stage	secno
Stage DC backup/tray spacing	TRATE-PANELB	DC-FLOOD	stage	secno
Stage DC velocity	TRATE-PANELB	DCV	stage	secno
Stage DC velocity/design velocity †††	TRATE-PANELB	DCV-FLOOD	stage	secno
Stage pressure drop	TRATE-PANELB	DP	stage	secno

† You can also access all block result variables for RADFRAC using the VECTOR-DEF sentence. See Chapter 29.

††† Not available for bubble cap and sieve trays.

continued

Tray rating results for panel C:

Description	Sentence	Variable†	ID1	ID2
Stage flooding factor	TRATE-PANELC	FLOOD-FAC	stage	secno
Stage DC backup	TRATE-PANELC	DCBA	stage	secno
Stage DC backup/tray spacing	TRATE-PANELC	DC-FLOOD	stage	secno
Stage DC velocity	TRATE-PANELC	DCV	stage	secno
Stage DC velocity/design velocity†††	TRATE-PANELC	DCV-FLOOD	stage	secno
Stage pressure drop	TRATE-PANELC	DP	stage	secno

Tray rating results for panel D:

Description	Sentence	Variable†	ID1	ID2
Stage flooding factor	TRATE-PANELD	FLOOD-FAC	stage	secno
Stage DC backup	TRATE-PANELD	DCBA	stage	secno
Stage DC backup/tray spacing	TRATE-PANELD	DC-FLOOD	stage	secno
Stage DC velocity	TRATE-PANELD	DCV	stage	secno
Stage DC velocity/design velocity†††	TRATE-PANELD	DCV-FLOOD	stage	secno
Stage pressure drop	TRATE-PANELD	DP	stage	secno

Packing sizing results:

Description	Sentence	Variable†	ID1	ID2
Column section diameter	PSIZE-RESULT	DIAM	secno	—
Limiting fractional approach to maximum capacity	PSIZE-RESULT	FLOOD-FAC	secno	—
Section pressure drop	PSIZE-RESULT	DPSEC	secno	—
Maximum liquid holdup for the section	PSIZE-HOLDUP	HOLDUP-MAX	secno	—
Stage fractional approach to maximum capacity	PSIZE-PROFILE	FLOOD-FAC	stage	secno
Stage pressure drop	PSIZE-PROFILE	DP	stage	secno
Stage HETP	PSIZE-PROFILE	HETP	stage	secno
Stage liquid holdup	PSIZE-HT-PROF	HOLDUP	stage	secno

Packing rating results:

Description	Sentence	Variable†	ID1	ID2
Limiting fractional approach to maximum capacity	PRATE-RESULT	FLOOD-FAC	secno	—
Section pressure drop	PRATE-RESULT	DPSEC	secno	—
Maximum liquid holdup for the section	PRATE-HOLDUP	HOLDUP-MAX	secno	—
Stage fractional approach to maximum capacity	PRATE-PROFILE	FLOOD-FAC	stage	secno
Stage pressure drop	PRATE-PROFILE	DP	stage	secno
Stage HETP	PRATE-PROFILE	HETP	stage	secno
Stage liquid holdup	PRATE-HT-PROF	HOLDUP	stage	secno

† You can also access all block result variables for RADFRAC using the VECTOR-DEF sentence. See Chapter 29.

††† Not available for bubble cap and sieve trays.

Accessing Variables in MULTIFRAC

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	Element
TRAY-SIZE	STAGE1, STAGE2, NPASS, TRAY-SPACE, FLOOD-FAC, SYSFAC, SLOT-AREA, HOLE-AREA, MIN-DIAM, MIN-DCAREA, OVER-DESIGN	secno	—
TRAY-RATE	STAGE1, STAGE2, NPASS, TRAY-SPACE, DIAM, SYSFAC, OVER-DESIGN, EFF, DECK-THICK, WEIR-HT-A, WEIR-HT-B, WEIR-HT-C, WEIR-HT-D, DC-CLEAR-SIDE, DC-CLEAR-CTR, DC-CLEAR-OFC, DC-WTOP-SIDE, DC-WTOP-CTR, DC-WTOP-OFC, DC-WBOT-SIDE, DC-WBOT-CTR, DC-WOT-OFC, DC-HT-SIDE, DC-HT-CTR, DC-HT-OFC, DC-OFC-WALL, CAP-DIAM, CAP-SPACE, SKIRT-HT, HOLE-DIAM, HOLE-AREA, VALVE-DEN, VALVE-THICK, VALVE-LIFT, DC-RTIME	secno	—
TRAY-RATE	NCAPS, NROWS, NVALVES	secno	†
PACK-SIZE	STAGE1, STAGE2, PACK-FAC, SPAREA, VOIDFR, STICH1, STICH2, STICH3, SYSFAC, OVER-DESIGN, PACK-HT, HETP, PACK-THICK, CS-APP, CS-FLOOD, CS-DESIGN, DPMAX-SEC, DPMAX-PACK	secno	—
PACK-RATE	STAGE1, STAGE2, PACK-FAC, SPAREA, VOIDFR, STICH1, STICH2, STICH3, SYSFAC, OVER-DESIGN, PACK-HT, HETP, DIAM, PACK-THICK, CS-FLOOD	secno	—

† Position in which you enter the variable. For variables in panels A through D, enter 1 through 4 for the elements .

Block Results

Hydraulic parameters:

Description	Sentence	Variable†	ID1††	ID2
Liquid mass flow from stage	HYDRAULIC	L-MASSFLOW	stack stage	—
Vapor mass flow to stage	HYDRAULIC	V-MASSFLOW	stack stage	—
Liquid volume flow from stage	HYDRAULIC	L-VOLFLOW	stack stage	—
Vapor volume flow to stage	HYDRAULIC	V-VOLFLOW	stack stage	—
Density of liquid from stage	HYDRAULIC	RHOL	stack stage	—
Density of vapor to stage	HYDRAULIC	RHOV	stack stage	—
Viscosity of liquid from stage	HYDRAULIC	MUL	stack stage	—

† You can also access all block result variables for MULTIFRAC using the VECTOR-DEF sentence. See Chapter 29.

†† Stack stage is the stage number if the columns are stacked one on top of another, starting with column 1. For example, if there are two columns and column 1 has 10 stages, stage 5 in column 2 has a stack stage number of 15.

continued

Hydraulic parameters (continued)

Description	Sentence	Variable†	ID1	ID2
Viscosity of vapor to stage	HYDRAULIC	MUV	stack stage	—
Surface tension of liquid from stage	HYDRAULIC	SIGMA	stack stage	—
Flow parameter	HYDRAULIC	FLOWPA	stack stage	—
Reduced vapor throughput	HYDRAULIC	QR	stack stage	—

Tray sizing results:

Description	Sentence	Variable†	ID1	ID2
Column section diameter	TSIZE-RESULT	DIAM	secno	—

Tray rating results:

Description	Sentence	Variable†	ID1	ID2
Maximum flooding factor	TRATE-RESULT	FLOOD-FAC	secno	—
Stage with maximum flooding factor	TRATE-RESULT	FLOOD-MAX	secno	—
Maximum downcomer backup	TRATE-RESULT	DCBA	secno	—
Maximum DC backup/tray spacing	TRATE-RESULT	DC-FLOOD	secno	—
Stage with maximum DC backup	TRATE-RESULT	DCBA-MAX	secno	—
Maximum downcomer velocity	TRATE-RESULT	DCV	secno	—
Stage with maximum DC velocity	TRATE-RESULT	DCV-MAX	secno	—
Section pressure drop	TRATE-RESULT	DPSEC	secno	—

Tray rating results for panel A:

Description	Sentence	Variable†	ID1††	ID2
Stage flooding factor	TRATE-PANELA	FLOOD-FAC	stack stage	secno
Stage DC backup	TRATE-PANELA	DCBA	stack stage	secno
Stage DC backup/tray spacing	TRATE-PANELA	DC-FLOOD	stack stage	secno
Stage DC velocity	TRATE-PANELA	DCV	stack stage	secno
Stage DC velocity/design velocity†††	TRATE-PANELA	DCV-FLOOD	stack stage	secno
Stage pressure drop	TRATE-PANELA	DP	stack stage	secno

Tray rating results for panel B:

Description	Sentence	Variable†	ID1	ID2
Stage flooding factor	TRATE-PANELB	FLOOD-FAC	stack stage	secno
Stage DC backup	TRATE-PANELB	DCBA	stack stage	secno
Stage DC backup/tray spacing	TRATE-PANELB	DC-FLOOD	stack stage	secno
Stage DC velocity	TRATE-PANELB	DCV	stack stage	secno
Stage DC velocity/design velocity†††	TRATE-PANELB	DCV-FLOOD	stack stage	secno
Stage pressure drop	TRATE-PANELB	DP	stack stage	secno

† You can also access all block result variables for MULTIFRAC using the VECTOR-DEF sentence. See Chapter 29.

†† Stack stage is the stage number if the columns are stacked one on top of another, starting with column 1. For example, if there are two columns and column 1 has 10 stages, stage 5 in column 2 has a stack stage number of 15.

continued

Tray rating results for panel C:

Description	Sentence	Variable†	ID1††	ID2
Stage flooding factor	TRATE-PANELC	FLOOD-FAC	stack stage	secno
Stage DC backup	TRATE-PANELC	DCBA	stack stage	secno
Stage DC backup/tray spacing	TRATE-PANELC	DC-FLOOD	stack stage	secno
Stage DC velocity	TRATE-PANELC	DCV	stack stage	secno
Stage DC velocity/design velocity†††	TRATE-PANELC	DCV-FLOOD	stack stage	secno
Stage pressure drop	TRATE-PANELC	DP	stack stage	secno

Tray rating results for panel D:

Description	Sentence	Variable†	ID1	ID2
Stage flooding factor	TRATE-PANELD	FLOOD-FAC	stack stage	secno
Stage DC backup	TRATE-PANELD	DCBA	stack stage	secno
Stage DC backup/tray spacing	TRATE-PANELD	DC-FLOOD	stack stage	secno
Stage DC velocity	TRATE-PANELD	DCV	stack stage	secno
Stage DC velocity/design velocity†††	TRATE-PANELD	DCV-FLOOD	stack stage	secno
Stage pressure drop	TRATE-PANELD	DP	stack stage	secno

Packing sizing results:

Description	Sentence	Variable†	ID1	ID2
Column section diameter	PSIZE-RESULT	DIAM	secno	—
Limiting fractional approach to maximum capacity	PSIZE-RESULT	FLOOD-FAC	secno	—
Section pressure drop	PSIZE-RESULT	DPSEC	secno	—

Packing rating results:

Description	Sentence	Variable†	ID1	ID2
Maximum liquid holdup for the section	PSIZE-HOLDUP	HOLDUP-MAX	secno	—
Stage fract. approach to maximum capacity	PSIZE-PROFILE	FLOOD-FAC	stack stage	secno
Stage pressure drop	PSIZE-PROFILE	DP	stack stage	secno
Stage HETP	PSIZE-PROFILE	HETP	stack stage	secno
Stage liquid holdup	PSIZE-HT-PROF	HOLDUP	stack stage	secno
Limiting fract. approach to maximum capacity	PRATE-RESULT	FLOOD-FAC	secno	—
Section pressure drop	PRATE-RESULT	DPSEC	secno	—
Maximum liquid holdup for the section	PRATE-HOLDUP	HOLDUP-MAX	secno	—
Stage fract. approach to maximum capacity	PRATE-PROFILE	FLOOD-FAC	stack stage	secno
Stage pressure drop	PRATE-PROFILE	DP	stack stage	secno
Stage HETP	PRATE-PROFILE	HETP	stack stage	secno
Stage liquid holdup	PRATE-HT-PROF	HOLDUP	stack stage	secno

† You can also access all block result variables for MULTIFRAC using the VECTOR-DEF sentence. See Chapter 29.

†† Stack stage is the stage number if the columns are stacked one on top of another, starting with column 1. For example, if there are two columns and column 1 has 10 stages, stage 5 in column 2 has a stack stage number of 15.

††† Not available for bubble cap and sieve trays.

Accessing Variables in PETROFRAC

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	ID2	Element
TRAY-SIZE	STAGE1, STAGE2, NPASS TRAY-SPACE, FLOOD-FAC, SYSFAC, SLOT-AREA, HOLE-AREA, MIN-DIAM, MIN-DCAREA, OVER-DESIGN	secno	—	—
TRAY-RATE	STAGE1, STAGE2, NPASS, TRAY-SPACE, DIAM, SYSFAC, OVER-DESIGN, EFF, DECK-THICK, WEIR-HT-A, WEIR-HT-B, WEIR-HT-C, WEIR-HT-D, DC-CLEAR-SIDE, DC-CLEAR-CTR, DC-CLEAR-OFC, DC-WTOP-SIDE, DC-WTOP-CTR, DC-WTOP-OFC, DC-WBOT-SIDE, DC-WBOT-CTR, DC-WOT-OFC, DC-HT-SIDE, DC-HT-CTR, DC-HT-OFC, DC-OFC-WALL, CAP-DIAM, CAP-SPACE, SKIRT-HT, HOLE-DIAM, HOLE-AREA, VALVE-DEN,VALVE-THICK, VALVE-LIFT, DC-RTIME	secno	—	—
TRAY-RATE	NCAPS, NROWS, NVALVES	secno	—	†
PACK-SIZE	STAGE1, STAGE2, PACK-FAC, SPAREA, VOIDFR, STICH1, STICH2, STICH3, SYSFAC, OVER-DESIGN, PACK-HT, HETP, PACK-THICK, CS-APP, CS-FLOOD, CS-DESIGN, DPMAX-SEC, DPMAX-PACK	secno	—	—
PACK-RATE	STAGE1, STAGE2, PACK-FAC, SPAREA, VOIDFR, STICH1, STICH2, STICH3, SYSFAC, OVER-DESIGN, PACK-HT, HETP, DIAM, PACK-THICK, CS-FLOOD	secno	—	—
STR-TRAY-SIZE	STAGE1, STAGE2, NPASS, TRAY-SPACE, FLOOD-FAC, SYSFAC, SLOT-AREA, HOLE-AREA, MIN-DIAM, MIN-DCAREA, OVER-DESIGN	stripid	secno	—
STR-TRAY-RATE	STAGE1, STAGE2, NPASS, TRAY-SPACE, DIAM, SYSFAC, OVER-DESIGN, EFF, DECK-THICK, WEIR-HT-A, WEIR-HT-B, WEIR-HT-C, WEIR-HT-D, DC-CLEAR-SIDE, DC-CLEAR-CTR, DC-CLEAR-OFC, DC-WTOP-SIDE, DC-WTOP-CTR, DC-WTOP-OFC, DC-WBOT-SIDE, DC-WBOT-CTR, DC-WOT-OFC, DC-HT-SIDE, DC-HT-CTR, DC-HT-OFC, DC-OFC-WALL, CAP-DIAM, CAP-SPACE, SKIRT-HT, HOLE-DIAM, HOLE-AREA, VALVE-DEN, VALVE-THICK, VALVE-LIFT, DC-RTIME	stripid	secno	—
STR-TRAY-RATE	NCAPS, NROWS, NVALVES	stripid	secno	†
STR-PACK-SIZE	STAGE1, STAGE2, PACK-FAC, SPAREA, VOIDFR, STICH1, STICH2, STICH3, SYSFAC, OVER-DESIGN, PACK-HT, HETP, PACK-THICK, CS-APP, CS-FLOOD, CS-DESIGN, DPMAX-SEC, DPMAX-PACK	stripid	secno	—
STR-PACK-RATE	STAGE1, STAGE2, PACK-FAC, SPAREA, VOIDFR, STICH1, STICH2, STICH3, SYSFAC, OVER-DESIGN, PACK-HT, HETP, DIAM, PACK-THICK, CS-FLOOD	stripid	secno	—

† Element is the position in which you enter the variable. For variables in panels A through D, enter 1 through 4 for the elements.

Block Results

Hydraulic parameters:

Description	Sentence	Variable†	ID1	ID2
Liquid mass flow from stage	HYDRAULIC	L-MASSFLOW	stage	—
Vapor mass flow to stage	HYDRAULIC	V-MASSFLOW	stage	—
Liquid volume flow from stage	HYDRAULIC	L-VOLFLOW	stage	—
Vapor volume flow to stage	HYDRAULIC	V-VOLFLOW	stage	—
Density of liquid from stage	HYDRAULIC	RHOL	stage	—
Density of vapor to stage	HYDRAULIC	RHOV	stage	—
Viscosity of liquid from stage	HYDRAULIC	MUL	stage	—
Viscosity of vapor to stage	HYDRAULIC	MUV	stage	—
Surface tension of liquid from stage	HYDRAULIC	SIGMA	stage	—
Flow parameter	HYDRAULIC	FLOWPA	stage	—
Reduced vapor throughput	HYDRAULIC	QR	stage	—

Tray sizing results:

Description	Sentence	Variable†	ID1	ID2
Column section diameter	TSIZE-RESULT	DIAM	secno	

Tray rating results:

Description	Sentence	Variable†	ID1	ID2
Maximum flooding factor	TRATE-RESULT	FLOOD-FAC	secno	
Stage with maximum flooding factor	TRATE-RESULT	FLOOD-MAX	secno	
Maximum downcomer backup	TRATE-RESULT	DCBA	secno	
Maximum downcomer backup/tray spacing	TRATE-RESULT	DC-FLOOD	secno	
Stage with maximum downcomer backup	TRATE-RESULT	DCBA-MAX	secno	
Maximum downcomer velocity	TRATE-RESULT	DCV	secno	
Stage with maximum downcomer velocity	TRATE-RESULT	DCV-MAX	secno	
Section pressure drop	TRATE-RESULT	DPSEC	secno	

Tray rating results for panel A:

Description	Sentence	Variable†	ID1	ID2
Stage flooding factor	TRATE-PANELA	FLOOD-FAC	stage	secno
Stage downcomer backup	TRATE-PANELA	DCBA	stage	secno
Stage downcomer backup/tray spacing	TRATE-PANELA	DC-FLOOD	stage	secno
Stage downcomer velocity	TRATE-PANELA	DCV	stage	secno
Stage downcomer velocity/design velocity††	TRATE-PANELA	DCV-FLOOD	stage	secno
Stage pressure drop	TRATE-PANELA	DP	stage	secno

† You can also access all block result variables for PETROFRAC using the VECTOR-DEF sentence. See Chapter 29.

†† Not available for bubble cap and sieve trays.

continued

Tray rating results for panel B:

Description	Sentence	Variable†	ID1	ID2
Stage flooding factor	TRATE-PANELB	FLOOD-FAC	stage	secno
Stage downcomer backup	TRATE-PANELB	DCBA	stage	secno
Stage downcomer backup/tray spacing	TRATE-PANELB	DC-FLOOD	stage	secno
Stage downcomer velocity	TRATE-PANELB	DCV	stage	secno
Stage downcomer velocity/design velocity††	TRATE-PANELB	DCV-FLOOD	stage	secno
Stage pressure drop	TRATE-PANELB	DP	stage	secno

Tray rating results for panel C:

Description	Sentence	Variable†	ID1	ID2
Stage flooding factor	TRATE-PANELC	FLOOD-FAC	stage	secno
Stage downcomer backup	TRATE-PANELC	DCBA	stage	secno
Stage downcomer backup/tray spacing	TRATE-PANELC	DC-FLOOD	stage	secno
Stage downcomer velocity	TRATE-PANELC	DCV	stage	secno
Stage downcomer velocity/design velocity††	TRATE-PANELC	DCV-FLOOD	stage	secno
Stage pressure drop	TRATE-PANELC	DP	stage	secno

Tray rating results for panel D:

Description	Sentence	Variable†	ID1	ID2
Stage flooding factor	TRATE-PANELD	FLOOD-FAC	stage	secno
Stage downcomer backup	TRATE-PANELD	DCBA	stage	secno
Stage downcomer backup/tray spacing	TRATE-PANELD	DC-FLOOD	stage	secno
Stage downcomer velocity	TRATE-PANELD	DCV	stage	secno
Stage downcomer velocity/design velocity††	TRATE-PANELD	DCV-FLOOD	stage	secno
Stage pressure drop	TRATE-PANELD	DP	stage	secno

Packing sizing results:

Description	Sentence	Variable†	ID1	ID2
Column section diameter	PSIZE-RESULT	DIAM	secno	—
Limiting fractional approach to maximum capacity	PSIZE-RESULT	FLOOD-FAC	secno	—
Section pressure drop	PSIZE-RESULT	DPSEC	secno	—
Maximum liquid holdup for the section	PSIZE-HOLDUP	HOLDUP-MAX	secno	—
Stage fractional approach to maximum capacity	PSIZE-PROFILE	FLOOD-FAC	stage	secno
Stage pressure drop	PSIZE-PROFILE	DP	stage	secno
Stage HETP	PSIZE-PROFILE	HETP	stage	secno
Stage liquid holdup	PSIZE-HT-PROF	HOLDUP	stack stage	secno

† You can also access all block result variables for PETROFRAC using the VECTOR-DEF sentence. See Chapter 29.

†† Not available for bubble cap and sieve trays.

continued

Packing rating results:

Description	Sentence	Variable†	ID1	ID2
Limiting fractional approach to maximum capacity	PRATE-RESULT	FLOOD-FAC	secno	—
Section pressure drop	PRATE-RESULT	DPSEC	secno	—
Maximum liquid holdup for the section	PRATE-HOLDUP	HOLDUP-MAX	secno	—
Stage fractional approach to maximum capacity	PRATE-PROFILE	FLOOD-FAC	stage	secno
Stage pressure drop	PRATE-PROFILE	DP	stage	secno
Stage HETP	PRATE-PROFILE	HETP	stage	secno
Stage liquid holdup	PRATE-HT-PROF	HOLDUP	stack stage	secno

Stripper hydraulic parameters:

Description	Sentence	Variable†	ID1	ID2
Liquid mass flow from stage	STR-HYDRAULIC	L-MASSFLOW	stripid	stage
Vapor mass flow to stage	STR-HYDRAULIC	V-MASSFLOW	stripid	stage
Liquid volume flow from stage	STR-HYDRAULIC	L-VOLFLOW	stripid	stage
Vapor volume flow to stage	STR-HYDRAULIC	V-VOLFLOW	stripid	stage
Density of liquid from stage	STR-HYDRAULIC	RHOL	stripid	stage
Density of vapor to stage	STR-HYDRAULIC	RHOV	stripid	stage
Viscosity of liquid from stage	STR-HYDRAULIC	MUL	stripid	stage
Viscosity of vapor to stage	STR-HYDRAULIC	MUV	stripid	stage
Surface tension of liquid from stage	STR-HYDRAULIC	SIGMA	stripid	stage
Flow parameter	STR-HYDRAULIC	FLOWPA	stripid	stage
Reduced vapor throughput	STR-HYDRAULIC	QR	stripid	stage

Stripper tray sizing results:

Description	Sentence	Variable†	ID1	ID2
Column section diameter	STR-TSIZE-RES	DIAM	secno	—

Stripper tray rating results:

Description	Sentence	Variable†	ID1	ID2
Maximum flooding factor	STR-TRATE-RES	FLOOD-FAC	secno	—
Stage with maximum flooding factor	STR-TRATE-RES	FLOOD-MAX	secno	—
Maximum downcomer backup	STR-TRATE-RES	DCBA	secno	—
Maximum downcomer backup/tray spacing	STR-TRATE-RES	DC-FLOOD	secno	—
Stage with maximum downcomer backup	STR-TRATE-RES	DCBA-MAX	secno	—
Maximum downcomer velocity	STR-TRATE-RES	DCV	secno	—
Stage with maximum downcomer velocity	STR-TRATE-RES	DCV-MAX	secno	—
Section pressure drop	STR-TRATE-RES	DPSEC	secno	—

† You can also access all block result variables for PETROFRAC using the VECTOR-DEF sentence. See Chapter 29.

continued

Stripper tray rating results for panel A:

Description	Sentence	Variable†	ID1	ID2
Stage flooding factor	STR-TRATE-A	FLOOD-FAC	stage	secno
Stage downcomer backup	STR-TRATE-A	DCBA	stage	secno
Stage downcomer backup/tray spacing	STR-TRATE-A	DC-FLOOD	stage	secno
Stage downcomer velocity	STR-TRATE-A	DCV	stage	secno
Stage downcomer velocity/design velocity††	STR-TRATE-A	DCV-FLOOD	stage	secno
Stage pressure drop	STR-TRATE-A	DP	stage	secno

Stripper tray rating results for panel B:

Description	Sentence	Variable†	ID1	ID2
Stage flooding factor	STR-TRATE-B	FLOOD-FAC	stage	secno
Stage downcomer backup	STR-TRATE-B	DCBA	stage	secno
Stage downcomer backup/tray spacing	STR-TRATE-B	DC-FLOOD	stage	secno
Stage downcomer velocity	STR-TRATE-B	DCV	stage	secno
Stage downcomer velocity/design velocity††	STR-TRATE-B	DCV-FLOOD	stage	secno
Stage pressure drop	STR-TRATE-B	DP	stage	secno

Stripper tray rating results for panel C:

Description	Sentence	Variable†	ID1	ID2
Stage flooding factor	STR-TRATE-C	FLOOD-FAC	stage	secno
Stage downcomer backup	STR-TRATE-C	DCBA	stage	secno
Stage downcomer backup/tray spacing	STR-TRATE-C	DC-FLOOD	stage	secno
Stage downcomer velocity	STR-TRATE-C	DCV	stage	secno
Stage downcomer velocity/design velocity††	STR-TRATE-C	DCV-FLOOD	stage	secno
Stage pressure drop	STR-TRATE-C	DP	stage	secno

Stripper tray rating results for panel D:

Description	Sentence	Variable†	ID1	ID2
Stage flooding factor	STR-TRATE-D	FLOOD-FAC	stage	secno
Stage downcomer backup	STR-TRATE-D	DCBA	stage	secno
Stage downcomer backup/tray spacing	STR-TRATE-D	DC-FLOOD	stage	secno
Stage downcomer velocity	STR-TRATE-D	DCV	stage	secno
Stage downcomer velocity/design velocity††	STR-TRATE-D	DCV-FLOOD	stage	secno
Stage pressure drop	STR-TRATE-D	DP	stage	secno

† You can also access all block result variables for PETROFRAC using the VECTOR-DEF sentence. See Chapter 29.

†† Not available for bubble cap and sieve trays.

continued

Stripper packing sizing results:

Description	Sentence	Variable†	ID1	ID2
Column section diameter	STR-PSIZE-RES	DIAM	secno	—
Limiting fractional approach to maximum capacity	STR-PSIZE-RES	FLOOD-FAC	secno	—
Section pressure drop	STR-PSIZE-RES	DPSEC	secno	—
Maximum liquid holdup for the section	STR-PS-HOLDUP	HOLDUP-MAX	secno	—
Stage fractional approach to maximum capacity	STR-PSIZE-PROF	FLOOD-FAC	stage	secno
Stage pressure drop	STR-PSIZE-PROF	DP	stage	secno
Stage HETP	STR-PSIZE-PROF	HETP	stage	secno
Stage liquid holdup	STR-PS-HTPROF	HOLDUP	stage	secno

Stripper packing rating results:

Description	Sentence	Variable†	ID1	ID2
Limiting fractional approach to maximum capacity	STR-PRATE-RES	FLOOD-FAC	secno	—
Section pressure drop	STR-PRATE-RES	DPSEC	secno	—
Maximum liquid holdup for the section	STR-PR-HOLDUP	HOLDUP-MAX	secno	—
Stage fractional approach to maximum capacity	STR-PRATE-PROF	FLOOD-FAC	stage	secno
Stage pressure drop	STR-PRATE-PROF	DP	stage	secno
Stage HETP	STR-PRATE-PROF	HETP	stage	secno
Stage liquid holdup	STR-PR-HTPROF	HOLDUP	stage	secno

† You can also access all block result variables for PETROFRAC using the VECTOR-DEF sentence. See Chapter 29.

†† Not available for bubble cap and sieve trays.

Unit Conversion Options

Several unit options are available for pressure, pressure drop, pressure drop per unit height of packing, packing factor, and valve density. Table 16.1 summarizes these unit options.

Table 16.1 Unit Options for Column Design and Rating

Variables	Units keyword	SI	ENG	MET	Other unit options
Pressure	PRESSURE	N/SQM	PSI	ATM	LBF/SQFT, BAR, TORR, IN-WATER, KG/SQCM, MMHG, KPA, MM-WATER, MBAR, PSIG, ATMG, BARG, KG/SQCMG
Pressure drop	PDROP	N/SQM	PSI	ATM	LBF/SQFT, BAR, TORR, IN-WATER, KG/SQCM, MMHG, KPA, MM-WATER, MBAR
Pressure drop per unit height	PDROP-PER-HT	N/CUM	IN-WATER/FT	MM-WATER/M	MBAR/M, MMHG/FT
Packing factor	PACK-FAC	1/M	1/FT	1/M	
Valve density	INVERSEAREA	1/SQM	1/SQFT	1/SQM	

Reference Tables

This section contains the following tables for reference when you enter sizing and rating specifications for bubble-cap trays, and random and structured packings:

Table	Title
16.2	Dimensions for Standard Stainless Steel Bubble Cap Designs
16.3	Types, Materials and Sizes of MTL Random Packings
16.4	Types, Materials and Sizes of Norton Random Packings
16.5	Types, Materials and Sizes of Generic Random Packings
16.6	Types, Materials and Sizes of Koch Random Packings
16.7	Types, Materials and Sizes of Raschig Random Packings
16.8	Types of Structured Packings

Table 16.2 Dimensions for Standard Stainless Steel Bubble Cap Designs

	Nominal Cap Size		
Dimensions	**3 in.**	**4 in.**	**6 in.**
Cap Dimensions:			
U.S. standard gauge	16	16	16
Outer diameter (in.)	2.999	3.999	5.999
Inner diameter (in.)	2.875	3.875	5.875
Height overall (in.)	2.500	3.000	3.750
Number of slots	20	26	39
Type of slots	Trapezoidal	Trapezoidal	Trapezoidal
Bottom slot width (in.)	0.333	0.333	0.333
Top slot width (in.)	0.167	0.167	0.167
Slot height (in.)	1.000	1.250	1.500
Height shroud ring (in.)	0.250	0.250	0.250
Riser Dimensions:			
U.S. standard gauge	16	16	16
Outer diameter (in.)	1.999	2.624	3.999
Inner diameter (in.)	1.875	2.500	3.875
Height (in.) for 0.5-in. skirt height	2.250	2.500	2.750
Height (in.) for 1.0-in. skirt height	2.750	3.000	3.250
Height (in.) for 1.5-in. skirt height	3.250	3.500	3.750
Riserslot seal (in.)	0.500	0.500	0.500
Cap Areas (in.):			
Riser	2.65	4.80	11.68
Reversal	4.18	7.55	17.80
Annular	3.35	6.38	14.55
Slot	5.00	8.12	14.64
Cap	7.07	12.60	28.30
Area Ratios:			
Reversal/riser	1.58	1.57	1.52
Annular/riser	1.26	1.33	1.25
Slot/riser	1.89	1.69	1.25
Slot/cap	0.71	0.65	0.52

Table 16.3 Types, Materials, and Sizes of MTL Random Packings

Packtype	Description of Packing	Pack-mat	Pack-size†		
CMR	Cascade® mini-ring	PLASTIC	NO-0A, NO-0.5A, NO-1A, NO-1, NO-2A, NO-2, NO-3A		
CMR	Cascade mini-ring	METAL	NO-0P, NO-0.5P, NO-1P NO-1.5P, NO-2P, NO-3P NO-4P, NO-5P		
CMR	Cascade mini-ring	CERAMIC	NO-0, NO-0.5, NO-1X, NO-2X, NO-2, NO-3, NO-5, NO-7		
BERL	Berl saddle	CERAMIC	0.5-IN 1-IN 1.5-IN 2-IN	or or or or	13-MM 25-MM 38-MM 50-MM
INTX	Intalox saddle	CERAMIC	1-IN 1.5-IN 2-IN 3-IN	or or or or	25-MM 38-MM 50-MM 75-MM
PALL	Pall ring	METAL	0.625-IN 1-IN 1.5-IN 2-IN	or or or or	16-MM 25-MM 38-MM 50-MM
PALL	Pall ring	PLASTIC	1-IN 1.5-IN 2-IN 3-IN	or or or or	25-MM 38-MM 50-MM 75-MM
RASCHIG	Raschig ring	CERAMIC	0.5-IN 1-IN 1.5-IN 2-IN 3-IN	or or or or or	13-MM 25-MM 38-MM 50-MM 75-MM
RASCHIG	Raschig ring	METAL	0.5-IN 1-IN 1.5-IN 2-IN 3-IN	or or or or or	13-MM 25-MM 38-MM 50-MM 75-MM

† You must put quotes around size codes containing a decimal point.

Table 16.4 Types, Materials, and Sizes of Norton Random Packings

Packtype	Description of Packing	Pack-mat	Pack-size†		
BERL	Berl saddle	CERAMIC	0.25-IN	or	6-MM
			0.5-IN	or	13-MM
			0.75-IN	or	19-MM
			1-IN	or	25-MM
			1.5-IN	or	38-MM
			2-IN	or	50-MM
HYPAK	Hy-Pak	METAL	1-IN	or	25-MM
			1.5-IN	or	38-MM
			2-IN	or	50-MM
			3.5-in	or	90-MM
IMTP	Intalox Metal Tower Packing (IMTP)	METAL	0.625-IN	or	16-MM
			1-IN	or	25-MM
			1.5-IN	or	38-MM
			2-IN	or	50-MM
			3-IN	or	75-MM
INTX	Intalox saddle	CERAMIC	0.25-IN	or	6-MM
			0.375-IN	or	10-MM
			0.5-IN	or	13-MM
			0.75-IN	or	19-MM
			1-IN	or	25-MM
			1.5-IN	or	38-MM
			2-IN	or	50-MM
			3-IN	or	75-MM
PALL	Pall ring	PLASTIC	0.625-IN	or	16-MM
			1-IN	or	25-MM
			1.5-IN	or	38-MM
			2-IN	or	50-MM
			3.5-IN	or	90-MM
PALL	Pall ring	METAL	0.625-IN	or	16-MM
			1-IN	or	25-MM
			1.5-IN	or	38-MM
			2-IN	or	50-MM
			3.5-IN	or	90-MM
RASCHIG	Raschig ring	CERAMIC	0.25-IN	or	6-MM
			0.375-IN	or	10-MM
			0.5-IN	or	13-MM
			0.625-IN	or	16-MM
			0.75-IN	or	19-MM
			1-IN	or	25-MM
			1.25-IN	or	30-MM
			1.5-IN	or	38-MM
			2-IN	or	50-MM
			3-IN	or	75-MM
RASCHIG	Raschig ring	METAL-32	0.25-IN	or	6-MM
			0.375-IN	or	10-MM
			0.5-IN	or	13-MM
			0.625-IN	or	16-MM
			0.75-IN	or	19-MM
			1-IN	or	25-MM

† You must put quotes around size codes containing a decimal point.

continued

Table 16.4 Types, Materials, and Sizes of Norton Random Packings (cont.)

Packtype	Description of Packing	Pack-mat	Pack-size†		
RASCHIG	Raschig ring	METAL-16	0.5-IN	or	13-MM
			0.625-IN	or	16-MM
			0.75-IN	or	19-MM
			1-IN	or	25-MM
			1.25-IN	or	30-MM
			1.5-IN	or	38-MM
			2-IN	or	50-MM
			3-IN	or	75-MM
SNOWFLAKE	Intalox Snowflake plastic packing	PLASTIC	II		
SUPER-INTX	Super Intalox saddle	CERAMIC	1-IN	or	25-MM
			2-IN	or	50-MM
SUPER-INTX	Super Intalox saddle	PLASTIC	1-IN	or	25-MM
			2-IN	or	50-MM
			3.5-in	or	90-MM

† You must put quotes around size codes containing a decimal point.

Table 16.5 Types, Materials, and Sizes of Generic Random Packings

Packtype	Description of Packing	Pack-mat	Pack-size†		
BERL	Berl saddle	CERAMIC	0.25-IN	or	6-MM
			0.5-IN	or	13-MM
			0.75-IN	or	19-MM
			1-IN	or	25-MM
			1.5-IN	or	38-MM
			2-IN	or	50-MM
COIL	Coil pack	—			2-MM
					3-MM
					4-MM
DIXON	Dixon packing	—			1.5-MM
					3-MM
			0.25-IN	or	6-MM
			0.6-IN	or	15-MM
			0.875-IN	or	20-MM
			1-IN	or	25-MM
HELI	Heli pack	—	NO-1, NO-2, NO-3, NO-4		
HELIX	Helix	—			2-MM
					2.5-MM
					3-MM
					4-MM
					5-MM
HYPAK	Hy-Pak	METAL	NO-1, NO-2		
I-BALL	I-ball packing	—	1-IN	or	25-MM
			2-IN	or	50-MM
			4-IN	or	100-MM
INTX	Intalox saddle	CERAMIC	0.25-IN	or	6-MM
			0.5-IN	or	13-MM
			1-IN	or	25-MM
			1.5-IN	or	38-MM
			2-IN	or	50-MM
			3-IN	or	75-MM
INTX	Intalox saddle	METAL	1-IN	or	25-MM
			1.5-IN	or	38-MM
			2-IN	or	50-MM
			3-IN	or	75-MM
INTX	Intalox saddle	PLASTIC	1-IN	or	25-MM
			2-IN	or	50-MM
			3-IN	or	75-MM
LESCHIG	Leschig ring	CERAMIC	1-IN	or	25-MM
			1.5-IN	or	38-MM
			2-IN	or	50-MM
MCMAHON	McMahon packing	—	0.25-IN	or	6-MM
			0.375-IN	or	10-MM
			0.6-IN	or	15-MM
			0.875-IN	or	20-MM
			1-IN	or	25-MM

† You must put quotes around size codes containing a decimal point.

continued

Table 16.5 Types, Materials, and Sizes of Generic Random Packing (cont.)

Packtype	Description of Packing	Pack-mat	Pack-size†		
MESH	Mesh ring	—	1-IN	or	25-MM
			1.25-IN	or	30-MM
			2-IN	or	50-MM
			4-IN	or	100-MM
PALL	Pall ring	METAL	0.625-IN	or	16-MM
			1-IN	or	25-MM
			1.5-IN	or	38-MM
			2-IN	or	50-MM
			3.5-IN	or	90-MM
PALL	Pall ring	PLASTIC	0.625-IN	or	16-MM
			1-IN	or	25-MM
			1.5-IN	or	38-MM
			2-IN	or	50-MM
			3.5-IN	or	90-MM
RASCHIG	Raschig ring	CARBON	1-IN	or	25-MM
			1.5-IN	or	38-MM
			2-IN	or	50-MM
RASCHIG	Raschig ring	CERAMIC	0.25-IN	or	6-MM
			0.375-IN	or	10-MM
			0.5-IN	or	13-MM
			0.6-IN	or	15-MM
			0.75-IN	or	19-MM
			1-IN	or	25-MM
			1.375-IN	or	35-MM
			1.5-IN	or	38-MM
			1.6-IN	or	40-MM
			2-IN	or	50-MM
			3-IN	or	75-MM
RASCHIG	Raschig ring	METAL	0.75-IN	or	19-MM
			1-IN	or	25-MM
			1.5-IN	or	38-MM
			2-IN	or	50-MM
			3-IN	or	75-MM
SIGMA	Sigma packing	—	0.25-IN	or	6-MM
			0.375-IN	or	10-MM
			0.6-IN	or	15-MM
			0.875-IN	or	20-MM
			1-IN	or	25-MM

† You must put quotes around size codes containing a decimal point.

Table 16.6 Types, Materials, and Sizes of Koch Random Packings

Packtype	Description of Packing	Pack-mat	Pack-size
FLEXIRING	Koch Flexiring single-tab slotted ring	STEEL	0.625-IN 1-IN 1.5-IN 2-IN 3.5-IN
FLEXIRING	Koch Flexiring single-tab slotted ring	POLYLPROP	0.625-IN 1-IN 1.5-IN 2-IN 3.5-IN
HCKP	Koch HCKP multi-tab slotted ring	STEEL	30-MM 45-MM 60-MM 90-MM
FLEXIMAX	Koch Fleximax high performance	STEEL	200 300 400 700
FLEXISADDLE	Koch Flexisaddle	POLYPROP	1-IN 2-IN 3-IN
FLEXISADDLE	Koch Flexisaddle	CERAMIC	0.75-IN 1-IN 1.5-IN 2-IN 3-IN

Table 16.7 Types, Materials, and Sizes of Raschig Random Packings

Packtype	Description of Packing	Pack-mat	Pack-size
SUPER-RING	Raschig Super-Ring	PLASTIC	0.6, 2
		METAL	0.3, 0.5, 0.7, 1, 1.5, 2, 3,
RALU-RING	Raschig Ralu-Ring	PLASTIC	15, 25, 38, 50, 90, 125
		METAL	25, 38, 50
PALL	Pall ring	PLASTIC	15, 25, 35, 50, 90
		METAL	15, 25, 35, 38, 50, 80
		CERAMIC	25, 35, 50
RASCHIG	Raschig Ring	METAL	15, 25, 35, 50
		CERAMIC	15, 25, 35, 50
RALU-FLOW	Raschig Ralu-Flow	PLASTIC	1, 2
RALU-PAK	Raschig Ralu-Pak	METAL	250YC
TORUSSADDL	Raschig Torus-Saddle	CERAMIC	1-IN, 1.5-IN, 2-IN
STORUSSDDL	Raschig Super-Torus-Saddle	PLASTIC	1-IN, 2-IN, 3-IN

Table 16.8 Types of Structured Packings

Packtype	Description of Packing	Pack-mat	Pack-size
GOODLOE	Glitsch Goodloe	STANDARD	—
GRID	Glitsch Grid	STANDARD	—
CY	Sulzer CY	STANDARD	STANDARD
KERAPAK	Sulzer Kerapak	STANDARD	STANDARD
MELLAPAK	Sulzer Mellapak	STANDARD	125X, 125Y, 170Y, 250X, 250Y, 350X, 350Y, 500X, 500Y, 750X, 750Y
BX	Sulzer BX	STANDARD	STANDARD
ISP	Norton Intalox	METAL	1T, 2T, 3T, 4T, 5T
FLEXIPAC	Koch Flexipac corrugated sheet	POLYPROP	2Y
FLEXIPAC	Koch Flexipac corrugated sheet	STEEL	1X, 1Y, 1.4X, 1.6Y, 2X, 2Y, 2.5Y, 3X, 3Y, 4Y
FLEXERAMIC	Koch Flexeramic	CERAMIC	28, 48, 88
FLEXIGRID	Koch Flexigrid	STEEL	STYLE-2, STYLE-3
SHEET-PACK	Raschig or generic sheet type structured packing	METAL	250Y, 350Y, 250X, 250Y-HC
WIRE-PACK	Raschig wire type structured packing	METAL	500Y
GRID-PACK	Raschig or generic grid type structured packing	METAL	P40Y, P64Y, P64X, P90X
SUPER-PAK	Raschig or generic Super-Pak	METAL	300
CROSSFLGRD	Raschig Cross-Flow-Grid	METAL	25, 50

17 Rate-Based Distillation

This chapter describes the input language used with RADFRAC for the RateSep rate-based distillation feature. RateSep requires a separate license, and can be used only by customers who have licensed it through a specific license agreement with Aspen Technology, Inc.

See also Chapter 15 for general input language for RADFRAC, and Chapter 16 for input language used for rating and sizing calculations for trays and packing.

Rate-Based Distillation in RADFRAC

Input Language for RADFRAC

```
BLOCK    blockid    RADFRAC
                .
                .
                .
RATESEP-ENAB    CALC-MODE=value
RATESEP-PARA    keyword=value
```

Optional keywords:

CC-AVG-PARAM RBTRFC RBRXN RBPACKEND INIT-EQUIL RS-TOL RS-MAXIT RS-STABLE-IT RS-STABLE-ME RS-X-TRANS RS-Y-TRANS CONTIN-ITER CONTIN-PAR DIAG-ITER DIAG-PROF RS-DTMAX NUMJAC EQUIL-FORM CHEM-RESTART FSCALE-EXP FUNC-RELAX

```
TRAY-REPORT    BUBBLE-DEW=value
TRAY-REPORT2   keyword=value
```

Optional keywords:

COMP-EFF STAGE-EFF MURPH-COMPS NTU-COMPS

```
PACK-RATE2    secno    keyword=value
```

Optional keywords:

RATE-BASED LIQ-FILM VAP-FILM LIQ-CORRF VAP-CORRF MTRFC-CORR HTRFC-CORR INTFA-CORR HOLDUP-CORR AREA-FACTOR MOLE-VHLDP MASS-VHLDP VOL-VHLDP MOLE-LHLDP MASS-LHLDP VOL-LHLDP PERCENT-VHLD PERCENT-LHLD VHLDP-FACTOR LHLDP-FACTOR NVPOINTS NLPOINTS VDISCPT LDISCPT BASE-STAGE BASE-FLOOD BILLET-CL BILLET-CV PACKING-SIZE PACK-TENSION STRUCT-BASE STRUCT-SIDE STRUCT-HEIGH S-ENHANCE-F S-RENEWAL-F U-MTRC-NUM U-HTRC-NUM U-IFAC-NUM U-HLDC-NUM FLOW-MODEL

```
TRAY-RATE2    secno    keyword=value
```

Optional keywords:

RATE-BASED LIQ-FILM VAP-FILM LIQ-CORRF VAP-CORRF MTRFC-CORR HTRFC-CORR INTFA-CORR HOLDUP-CORR AREA-FACTOR MOLE-VHLDP MASS-VHLDP VOL-VHLDP MOLE-LHLDP MASS-LHLDP VOL-LHLDP RATIO-VSPACE VHLDP-FACTOR LHLDP-FACTOR NVPOINTS NLPOINTS VDISCPT LDISCPT BASE-STAGE BASE-FLOOD HOLE-PITCH U-MTRC-NUM U-HTRC-NUM U-IFAC-NUM U-HLDC-NUM FLOW-MODEL FLOWPATH-FCT DC-RES-TIME

SUBROUTINE *keyword=value*

Keywords:

SUB-MTRC SUB-HTRC SUB-IFAC SUB-HLDC

MTRFC-VECS **NINT**=*value* **NREAL**=*value*
MTRFC-INT **VALUE=LIST**=*values*
MTRFC-REAL **VALUE=LIST**=*values*
HTRFC-VECS **NINT**=*value* **NREAL**=*value*
HTRFC-INT **VALUE=LIST**=*values*
HTRFC-REAL **VALUE=LIST**=*values*
INTFA-VECS **NINT**=*value* **NREAL**=*value*
INTFA-INT **VALUE=LIST**=*values*
INTFA-REAL **VALUE=LIST**=*values*
HOLDUP-VECS **NINT**=*value* **NREAL**=*value*
HOLDUP-INT **VALUE=LIST**=*values*
HOLDUP-REAL **VALUE=LIST**=*values*

Input Language Description for RADFRAC

RATESEP-ENAB Use to turn on the RateSep capability which can model non-equilibrium stages. A RateSep license is needed to run a RadFrac model with this feature.

CALC-MODE..... Use to specify the calculation mode.

CALC-MODE= EQUILIBRIUM	All inputs related to RateSep are ignored and RadFrac operates in equlibrium stage mode. (Default)
CALC-MODE=RIG-RATE	RateSep functionality is enabled. There must be at least one rate-based Tray Rating or Pack Rating section. Stages in such a rate-based Rating section are treated as rate-based; all other stages are treated as equilibrium-based. Use the TRAY-RATE2 and PACK-RATE2 sentences to specify these rate-based Rating sections.

RATESEP-PARA Use to specify parameters used in rate-based calculations.

CC-AVG-PARAM..... Weighting parameter used for average diffusivity and average binary mass transfer coefficient calculations for the Chilton-Colburn analogy. The following formula is used:

$$\overline{Z}_j = \frac{\sum_{i=1}^{nc-1}\sum_{k=i+1}^{nc}\left(x_{ij}+\delta\right)\left(x_{kj}+\delta\right)Z_{ikj}}{\sum_{i=1}^{nc-1}\sum_{k=i+1}^{nc}\left(x_{ij}+\delta\right)\left(x_{kj}+\delta\right)}$$

where Z is the property being averaged, j is the stage number, nc is the number of components, and δ is this parameter. A large value will diminish the impact of compositions. (Default = 0.0001)

RBTRFC..... Weighting factor for conditions (T and x) used to calculate mass transfer coefficients. The condition used is calculated by:

$$Z_{used} = \delta Z_{bulk} + (1-\delta)Z_{interface}$$

where δ is this parameter. (Default = 0.5)

RBRXN ..... Weighting factor for conditions (T and x) used to calculate film reaction rates. The condition used is calculated by:

$$Z_{used} = \delta Z_{bulk} + (1-\delta) Z_{interface}$$

where δ is this parameter. (Default = 0.5)

RBPACKEND ..... Weighting factor for conditions (T and x) used to calculate flux and reaction extents for top and bottom stages. Values are calculated by:

$$Z_{used} = \delta Z_{end} + (1-\delta) Z_{internal}$$

where δ is this parameter. (Default = 0.5)

INIT-EQUIL..... Equilibrium initialization flag.

INIT-EQUIL=YES	The equilibrium solution is used to initialize rate-based calculations. (Default)
INIT-EQUIL=NO	Equilibrium calculations are skipped and rate-based calculations are initialized from estimates of stage temperatures and compositions.

RS-TOL..... When root-mean-square residual is less than this tolerance, the RateSep rate-based column calculations are considered to be converged. (Default = 1.0 x 10^{-5})

Note: During the equilibrium-based initialization calculations, the convergence parameters from the PARAM sentence are used instead.

RS-MAXIT ..... Maximum number of iterations for rate-based calculations. (Default=25)

RS-STABLE-IT ..... Initial number of stabilization iterations when using the dogleg strategy or line search for rate-based calculations. (Default = 0)

RS-STABLE-ME ..... Stabilization method for rate-based calculations. (Default = the method specified for STABLE-METH in the CONVERGENCE sentence for equilibrium calculations, or LINE-SEARCH if that is unspecified.)

RS-STABLE-ME=DOGLEG	Dogleg method.
RS=STABLE-ME= LINE-SEARCH	Line search method.

RS-X-TRANS, RS-Y-TRANS..... Liquid (X) and vapor (Y) flow variable transformations for rate-based calculations. RateSep uses these transformations to aid convergence. In the transformations below, x is the variable and F(i,j) is the flow of component i in the phase being transformed on stage j.

...=LINEAR	x = F(i,j) (no transformation)
...=SQUARE	x = F(i,j) x F(i,j)
...=EXPONENTIAL	x = exp(F(i,j))
...=STANDARD	(Default) The first applicable case from the following list is applied: • Nonreactive systems: Linear • Extremely small component flows: Linear • Equilibrium reactions and small flows: Exponential • All other systems: Square

CONTIN-ITER Number of continuation/homotopy points iteration points for rate-based calculations. This many rate-based sub-problems are solved after the equilibrium-based initialization before the actual rate-based model is solved for the first time. The equilibrium solution is used as the starting point for the first sub-problem and each sub-problem's solution is used as the starting point for the next sub-problem. Used in conjunction with CONTIN-PAR. (Default=0)

CONTIN-PAR Initial parameter for continuation/homotopy method. For homotopy to be effective, this should be changed to a value larger than its 1.0 default which represents a jump directly to the actual rate-based problem. Larger values represent sub-problems closer to the equilibrium solution. The value of CONTIN-PAR is used for the first sub-problem. For subsequent subproblems, the value used is $(\text{CONTIN-PAR})^{(\text{-1/CONTIN-ITER})}$.

(Default=1.0)

DIAG-ITER Level of error and diagnostic messages printed in the history file for rate-based iterations. (Default = block simulation message level, SIM-LEVEL in BLOCK-OPTION sentence)

DIAG-PROF In rate-based calculations, controls printing of initial and final profiles to history file. (Default = block simulation message level, SIM-LEVEL in BLOCK-OPTION sentence)

RS-DTMAX Maximum allowed temperature change on any one stage from one rate-based iteration to the next. (Default = 15)

NUMJAC Jacobian matrix calculation option for rate-based simulations. (Default is based on PROP-DERIV in the CONVERGENCE sentence; NONE if PROP-DERIV is ANALYTICAL, PROPERTY if PROP-DERIV is NUMERICAL.

In apparent-composition systems, property derivatives are always computed numerically, regardless of this option.

NUMJAC=NONE	Use analytical derivatives whenever possible.
NUMJAC=PROPERTY	Compute property derivatives numerically.
NUMJAC=JACOBIAN	Compute Jacobian matrix by perturbation. Most (but not all) property derivatives are computed numerically.
NUMJAC=ALL	Compute all property derivatives and Jacobian matrix numerically.

EQUIL-FORM Equilibrium reaction formulation.

EQUIL-FORM=STANDARD	Standard formulation (Default)
EQUIL-FORM= LOGARITHMIC	Logarithmic formulation
EQUIL-FORM=PRODUCT	Product formulation

CHEM-RESTART Whether to use retention for Chemistry calculations using the apparent components approach.

CHEM-RESTART =YES	Use retention for Chemistry calculations using the apparent components approach. (Default)
CHEM-RESTART =NO	Do not use retention for Chemistry calculations using the apparent components approach.

FSCALE-EXP Additional scaling based on Jacobian elements. A value of 0.0 means no additional scaling. (Default=0.25)

FUNC-RELAX Maximum function error relaxation parameter. A value of 1.0 means no relaxation. (Default=20)

TRAY-REPORT Options for the tray report for rate-based simulations.

BUBBLE-DEW ..... Whether to report bubble and dew point temperature profiles.

BUBBLE-DEW=YES	Report bubble and dew point profiles.
BUBBLE-DEW=NO	Do not report bubble and dew point profiles. (Default)

TRAY-REPORT2 Additional options for the tray report for rate-based simulations.

COMP-EFF ..... Whether to report component-by-component Murphree vapor efficiency profiles for the components specified in MURPH-COMPS.

COMP-EFF=YES	Report component efficiency profiles.
COMP-EFF=NO	Do not report component efficiency profiles. (Default)

STAGE-EFF ..... Whether to report tray efficiency profile based on key components specified in NTU-COMPS.

STAGE-EFF=YES	Report tray efficiency profiles.
STAGE-EFF=NO	Do not report tray efficiency profiles. (Default)

MURPH-COMPS ..... Components whose efficiencies are to be reported (Default = all components)

NTU-COMPS ..... List of components forming the basis for the calculations of stage efficiency or the Height Equivalent to a Theoretical Plate (HETP). (Default = all components)

PACK-RATE2 Options for rate-based pack rating calculations. Rate-based tray rating and pack rating sections must not overlap among themselves or each other.

secno ..... Section number of a pack rating section. A PACK-RATE sentence for the same section must also be specified.

RATE-BASED ..... Whether the section is solved using rate-based calculations.

RATE-BASED=YES	The other parameters in this sentence are used to define the rate-based pack rating section.
RATE-BASED=NO	Equilibrium calculations are used in this section and the rest of this sentence is ignored. (Default)

LIQ-FILM, VAP-FILM ... Liquid and vapor film resistance options

…=NOFILM	No film resistance in this phase
…=FILM	Diffusion resistance but no reactions in film in this phase
…=FILMRXN	Diffusion resistance with reactions in film in this phase. (Default)
…=DISCRXN	Diffusion resistance with reactions in film in this phase. Film is discretized.

LIQ-CORRF, VAP-CORRF ..... Whether to apply film non-ideality correction for liquid film and vapor film.

…=YES	Apply non-ideality correction in this phase
…=NO	Do not apply non-ideality correction in this phase. (Default)

MTRFC-CORR..... Mass transfer coefficient correlation. Details about the correlations are available in the online help. Look for **Built-In Correlations** in the Index. Default correlation depends on packing type.

MTRFC-CORR=ONDA-68	Onda (1968) correlation for random packing
MTRFC-CORR= BRAVO-FAIR82	Bravo and Fair (1982) correlation for random packing
MTRFC-CORR=BILLET-93	Billet and Schultes (1983) correlation for all packing types

	MTRFC-CORR=BRF-85	Bravo, Rocha, and Fair (1985) correlation for structured packing
	MTRFC-CORR=BRF-92	Bravo, Rocha, and Fair (1992) correlation for structured packing
	MTRFC-CORR=USER	Correlation defined by user subroutine. Specify subroutine name in the SUBROUTINE sentence. See *Aspen Plus User Models* for details on writing the subroutine.
HTRFC-CORR	Heat transfer coefficient correlation. Details are available in the online help. Look for **Built-In Correlations** in the Index.	
	HTRFC-CORR= CHILTON-COLB	Method based on the Chilton-Colburn Analogy. (Default)
	HTRFC-CORR=USER	Correlation defined by user subroutine. Specify subroutine name in the SUBROUTINE sentence. See *Aspen Plus User Models* for details on writing the subroutine.
INTFA-CORR	Interfacial area correlation. Details about the correlations are available in the online help. Look for **Built-In Correlations** in the Index. Default correlation depends on packing type and mass transfer correlation selected.	
	INTFA-CORR=ONDA-68	Onda (1968) correlation for random packing
	INTFA-CORR= BRAVO-FAIR82	Bravo and Fair (1982) correlation for random packing
	INTFA-CORR=BILLET-93	Billet and Schultes (1983) correlation for all packing types
	INTFA-CORR=BRF-85	Bravo, Rocha, and Fair (1985) correlation for structured packing
	INTFA-CORR=BRF-92	Bravo, Rocha, and Fair (1992) correlation for structured packing
	INTFA-CORR=USER	Correlation defined by user subroutine. Specify subroutine name in the SUBROUTINE sentence. See *Aspen Plus User Models* for details on writing the subroutine.
HOLDUP-CORR	Holdup correlation for kinetic reactions. It is used when a phase has kinetic reactions and the holdup for that phase is not specified. Default correlation depends on packing type and correlations selected for mass transfer and interfacial area.	
	HOLDUP-CORR= STICHLMAIR89	Stichlmair, Bravo, and Fair (1989) correlation
	HOLDUP-CORR=BRF-92	Bravo, Rocha, and Fair (1992) correlation for structured packing
	HOLDUP-CORR= BILLET-93	Billet and Schultes (1983) correlation
	HOLDUP-CORR= PERCENT-DATA	Holdup calculated from specified percent liquid or percent vapor
	HOLDUP-CORR=USER	Correlation defined by user subroutine. Specify subroutine name in the SUBROUTINE sentence. See *Aspen Plus User Models* for details on writing the subroutine.
AREA-FACTOR	Scale factor for interfacial area for rate-based calculations. Interfacial area and transfer coefficients from correlations are multiplied by this factor. (Default=1)	
MOLE-VHLDP, MASS-VHLDP, VOL-VHLDP	Vapor holdup for vapor-phase kinetic reactions on a mole, mass, or volume basis. If specified, the holdup correlation is not used for vapor holdup.	

MOLE-LHLDP, MASS-LHLDP, VOL-LHLDP ..... Liquid holdup for liquid-phase kinetic reactions on a mole, mass, or volume basis. If specified, the holdup correlation is not used for liquid holdup.

PERCENT-VHLD ..... Vapor percent of free volume for vapor phase kinetic reactions. Can be more than 100%.

PERCENT-LHLD ..... Liquid percent of free volume for liquid phase kinetic reactions. Can be more than 100%.

PERCENT-VHLD and PERCENT-LHLD can be specified independently, and do not have to add up to 100%.

VHLDP-FACTOR LHLDP-FACTOR ..... Scale factors for vapor holdup and liquid holdup. Holdups (user-specified or calculated by correlation) are multiplied by these factors. (Default=1)

NVPOINTS, NLPOINTS Number of additional discretization points in the vapor film and liquid film, used when VAP-FILM or LIQ-FILM is DISCRXN. (Default=0)

VDISCPT, LDISCPT..... Locations of additional discretization points in the vapor film and liquid film. Points are always added at 0 (vapor-liquid interface) and 1 (bulk vapor or bulk liquid). Additional points should be specified in increasing order between 0 and 1.

Default is to allocate the additional discretization points evenly between 0 and 1. This is used whenever the locations for the points are not specified, the number of points specified does not match NVPOINTS or NLPOINTS, some points are missing (* in input file), points are not in monotonically increasing order, or the difference between two adjacent points is less than 10^{-6}.

BASE-STAGE ..... Base stage for column diameter calculation. When BASE-STAGE is specified, RateSep performs calculations in design mode for this section. The specified column diameter is used as an estimate.

There are restrictions on what stages can be used as BASE-STAGE. If there are no overlapping sections, the stage must be within this rate-based section. For more information, see **RateSep:Design calculation** in the Index of the online help.

BASE-FLOOD ..... Fractional approach to maximum capacity on base stage for column diameter calculation. (Default=0.8)

BILLET-CL, BILLET-CV. Billet and Schultes correlation parameters for liquid phase and vapor phase mass transfer.

PACKING-SIZE ..... Packing size for random packings. Used to override the value from the packing databank for the specified packing.

PACK-TENSION ..... Critical surface tension for the packing material. Used in the ONDA-68 interfacial area correlation and provided to user routines for mass transfer coefficients, interfacial area, and holdup.

Default depends on packing material. For PLASTIC or POLYPROP, 0.033 N/m. For CERAMIC, 0.061 N/m. For CARBON, 0.056 N/m. For other materials, 0.075 N/m.

STRUCT-BASE, STRUCT-SIDE, STRUCT-HEIGH ..... Base width, side dimension, and height of corrugation for structured packing, used with the BRF-85 and BRF-92 correlations. (BRF-92 only uses STRUCT-SIDE.)

S-ENHANCE-F, S-RENEWAL-F ..... Factor for surface enhancement and correction factor for surface renewal, used with the BRF-92 correlation.

U-MTRC-NUM ..... Mass transfer correlation number, used when MTRFC-CORR=USER.

U-HTRC-NUM..... Heat transfer correlation number, used when HTRFC-CORR=USER.

U-IFAC-NUM ..... Interfacial area correlation number, used when INTFA-CORR=USER.

U-HLDC-NUM ..... Holdup correlation number, used when HOLDUP-CORR=USER, the section involves kinetic reactions, and holdups are not specified.

You can implement multiple correlations in each of these four subroutines. These numbers are passed to the relevant subroutines to select which correlation is used.

FLOW-MODEL..... Flow pattern.

FLOW-MODEL=MIXED	Both liquid and vapor phases are well mixed. The bulk properties for each phase are assumed to be the same as the outlet conditions for that phase leaving that stage. (Default)
FLOW-MODEL= COUNTERCURRE	Liquid and vapor flow are countercurrent. The bulk properties for each phase are an average of the inlet and outlet properties. For example, $x_{i,avg} = \left(x_{i,j} + x_{i,j-1}\right)/2$ where i is the component index and j is the stage index.
FLOW-MODEL=VPLUG	Liquid phase is well mixed, vapor phase is plug flow. Outlet conditions are used for the bulk liquid and average conditions are used for the vapor, except that outlet pressure is used for both phases.
FLOW-MODEL= VPLUG-PAVG	Liquid phase is well mixed, vapor phase is plug flow. Outlet conditions are used for the bulk liquid and average conditions are used for the vapor, except that average pressure is used for both phases.

TRAY-RATE2 Options for rate-based tray rating calculations. Rate-based tray rating and pack rating sections must not overlap among themselves or each other.

secno ..... Section number of a tray rating section. A TRAY-RATE sentence for the same section must also be specified.

RATE-BASED ..... Whether the section is solved using rate-based calculations.

RATE-BASED=YES	The other parameters in this sentence are used to define the rate-based tray rating section.
RATE-BASED=NO	Equilibrium calculations are used in this section and the rest of this sentence is ignored. (Default)

LIQ-FILM, VAP-FILM ... Liquid and vapor film resistance options

…=NOFILM	No film resistance in this phase
…=FILM	Diffusion resistance but no reactions in film in this phase
…=FILMRXN	Diffusion resistance with reactions in film in this phase. (Default)
…=DISCRXN	Diffusion resistance with reactions in film in this phase. Film is discretized.

LIQ-CORRF, VAP-CORRF ..... Whether to apply film non-ideality correction for liquid film and vapor film.

…=YES	Apply non-ideality correction in this phase
…=NO	Do not apply non-ideality correction in this phase. (Default)

MTRFC-CORR..... Mass transfer coefficient correlation. Details about the correlations are available in the online help. Look for **Built-In Correlations** in the Index. Default correlation depends on tray type.

MTRFC-CORR=AICHE-58	AICHE (1958) correlation for all tray types
MTRFC-CORR= HUGHMARK-71	Hughmark (1971) correlation for bubble-cap trays
MTRFC-CORR= SCHEFFE-87	Scheffe and Weiland (1987) correlation for valve trays
MTRFC-CORR= CHAN-FAIR-84	Chan and Fair (1984) correlation for sieve trays
MTRFC-CORR= ZUIDERWEG-82	Zuiderweg (1982) correlation for sieve trays
MTRFC-CORR= CHENCHUANG93	Chen and Chuang correlation for sieve trays
MTRFC-CORR= GERSTER-85	Gerster at al. (1958) correlation for all tray types
MTRFC-CORR= CHAN-FAIR-RF	Implementation of the Chan and Fair (1984) correlation for sieve trays used in RateFrac. It uses Gerster for the liquid and Chan and Fair for the vapor.
MTRFC-CORR=USER	Correlation defined by user subroutine. Specify subroutine name in the SUBROUTINE sentence. See *Aspen Plus User Models* for details on writing the subroutine.

HTRFC-CORR..... Heat transfer coefficient correlation. Details are available in the online help. Look for **Built-In Correlations** in the Index.

HTRFC-CORR= CHILTON-COLB	Method based on the Chilton-Colburn Analogy. (Default)
HTRFC-CORR=USER	Correlation defined by user subroutine. Specify subroutine name in the SUBROUTINE sentence. See *Aspen Plus User Models* for details on writing the subroutine.

INTFA-CORR ..... Interfacial area correlation. Details about the correlations are available in the online help. Look for **Built-In Correlations** in the Index. Default correlation depends on tray type and mass transfer correlation selected.

INTFA-CORR= SCHEFFE-87	Scheffe and Weiland (1987) correlation for valve trays
INTFA-CORR= ZUIDERWEG-82	Zuiderweg (1982) correlation for sieve trays
INTFA-CORR=USER	Correlation defined by user subroutine. Specify subroutine name in the SUBROUTINE sentence. See *Aspen Plus User Models* for details on writing the subroutine.

HOLDUP-CORR..... Holdup correlation for kinetic reactions. It is used when a phase has kinetic reactions and the holdup for that phase is not specified. Default correlation depends on tray type and correlations selected for mass transfer and interfacial area.

HOLDUP-CORR= BENNETT-83	Bennett, Agrawal, and Cook (1983) correlation for sieve trays and extension for other tray types
HOLDUP-CORR= ZUIDERWEG-82	Zuiderweg (1982) correlation for sieve trays
HOLDUP-CORR= STICHLMAIR78	Stichlmair (1978) correlation
HOLDUP-CORR= PERCENT-DATA	Holdup calculated from specified percent liquid or percent vapor

HOLDUP-CORR=USER	Correlation defined by user subroutine. Specify subroutine name in the SUBROUTINE sentence. See *Aspen Plus User Models* for details on writing the subroutine.
AREA-FACTOR	Scale factor for interfacial area for rate-based calculations. Interfacial area and transfer coefficients from correlations are multiplied by this factor. (Default=1)
MOLE-VHLDP, MASS-VHLDP, VOL-VHLDP	Vapor holdup for vapor-phase kinetic reactions on a mole, mass, or volume basis. If specified, the holdup correlation is not used for vapor holdup.
MOLE-LHLDP, MASS-LHLDP, VOL-LHLDP	Liquid holdup for liquid-phase kinetic reactions on a mole, mass, or volume basis. If specified, the holdup correlation is not used for liquid holdup.
RATIO-VSPACE	Fraction of vapor space included in each tray's vapor holdup. Used in stages with vapor-phase kinetic reactions. Vapor holdup for trays consists of two parts, the vapor holdup in the froth on the tray floor and the vapor holdup outside the froth. The second part is calculated as the tray space not occupied by froth multiplied by RATIO-VSPACE.
VHLDP-FACTOR LHLDP-FACTOR	Scale factors for vapor holdup and liquid holdup. Holdups (user-specified or calculated by correlation) are multiplied by these factors. (Default=1)
NVPOINTS, NLPOINTS	Number of additional discretization points in the vapor film and liquid film, used when VAP-FILM or LIQ-FILM is DISCRXN. (Default=0)
VDISCPT, LDISCPT	Locations of additional discretization points in the vapor film and liquid film. Points are always added at 0 (vapor-liquid interface) and 1 (bulk vapor or bulk liquid). Additional points should be specified in increasing order between 0 and 1. Default is to allocate the additional discretization points evenly between 0 and 1. This is used whenever the locations for the points are not specified, the number of points specified does not match NVPOINTS or NLPOINTS, some points are missing (* in input file), points are not in monotonically increasing order, or the difference between two adjacent points is less than 10^{-6}.
BASE-STAGE	Base stage for column diameter calculation. When BASE-STAGE is specified, RateSep performs calculations in design mode for this section. The specified column diameter is used as an estimate. There are restrictions on what stages can be used as BASE-STAGE. If there are no overlapping sections, the stage must be within this rate-based section. For more information, see **RateSep:Design calculation** in the Index of the online help.
BASE-FLOOD	Fractional approach to maximum capacity on base stage for column diameter calculation. (Default=0.8)
HOLE-PITCH	Hole pitch for sieve trays. A warning will be issued if hole pitch specified is greater than 5 times hole diameter. (Default is calculated based on a triangular arrangement.)
U-MTRC-NUM	Mass transfer correlation number, used when MTRFC-CORR=USER.
U-HTRC-NUM	Heat transfer correlation number, used when HTRFC-CORR=USER.

U-IFAC-NUM ..... Interfacial area correlation number, used when INTFA-CORR=USER.

U-HLDC-NUM ..... Holdup correlation number, used when HOLDUP-CORR=USER, the section involves kinetic reactions, and holdups are not specified.

You can implement multiple correlations in each of these four subroutines. These numbers are passed to the relevant subroutines to select which correlation is used.

FLOW-MODEL..... Flow pattern.

FLOW-MODEL=MIXED	Both liquid and vapor phases are well mixed. The bulk properties for each phase are assumed to be the same as the outlet conditions for that phase leaving that stage. (Default)
FLOW-MODEL= COUNTERCURRE	Liquid and vapor flow are countercurrent. The bulk properties for each phase are an average of the inlet and outlet properties. For example, $x_{i,avg} = \left(x_{i,j} + x_{i,j-1}\right)/2$ where i is the component index and j is the stage index.
FLOW-MODEL=VPLUG	Liquid phase is well mixed, vapor phase is plug flow. Outlet conditions are used for the bulk liquid and average conditions are used for the vapor, except that outlet pressure is used for both phases.
FLOW-MODEL= VPLUG-PAVG	Liquid phase is well mixed, vapor phase is plug flow. Outlet conditions are used for the bulk liquid and average conditions are used for the vapor, except that average pressure is used for both phases.

FLOWPATH-FCT..... Average flow path mixing factor (A). Average flow path length is calculated as Z = (1-A)*Z0 + A*Z1 where Z0 is the distance straight across the tray and Z1 is the total bubbling area divided by the weir length and number of passes. (Default 0.5)

DC-RES-TIME ..... Liquid residence time in the downcomer. Used to calculated liquid holdup in the downcomer in systems with kinetic reactions in the liquid phase. The calculated liquid holdup is also scaled by LHLDP-FACTOR. (Default=0)

SUBROUTINE Use to specify names of user subroutines for correlations used in rate-based calculations when a TRAY-RATE2 or PACK-RATE2 section uses a USER correlation.

SUB-MTRC..... User subroutine name for mass transfer coefficients.

SUB-HTRC..... User subroutine name for heat transfer coefficients.

SUB-IFAC..... User subroutine name for interfacial area.

SUB-HLDC..... User subroutine name for holdup.

MTRFC-VECS, HTRFC-VECS, INTFA-VECS, HOLDUP-VECS Use to specify the number of integer and real parameters for user subroutines for mass transfer (MTRFC), heat transfer (HTRFC), interfacial area (INTFA), and holdup (HOLDUP).

NINT..... Number of integer parameters for user subroutine (Default=1)

NREAL..... Number of real parameters for user subroutine (Default=1)

MTRFC-INT, HTRFC-INT, INTFA-INT, HOLDUP-INT Use to specify the integer parameters for user subroutines for mass transfer (MTRFC), heat transfer (HTRFC), interfacial area (INTFA), and holdup (HOLDUP).

VALUE-LIST ..... Vector of parameters passed into user subroutine

MTRFC-REAL, HTRFC-REAL, INTFA-REAL, HOLDUP-REAL

Use to specify the real parameters for user subroutines for mass transfer (MTRFC), heat transfer (HTRFC), interfacial area (INTFA), and holdup (HOLDUP).

VALUE-LIST ..... Vector of parameters passed into user subroutine

Accessing Variables in RADFRAC

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	Element
RATESEP-PARA	RBTRFC, RBRXN, RBPACKEND, CC-AVG-PARAM	—	—
PACK-RATE2	AREA-FACTOR, MOLE-VHLDP, MASS-VHLDP, VOL-VHLDP, MOLE-LHLDP, MASS-LHLDP, VOL-LHLDP, PERCENT-VHLD, PERCENT-LHLD, VHLDP-FACTOR, LHLDP-FACTOR, BASE-STAGE, BASE-FLOOD, BILLET-CL, BILLET-CV, PACKING-SIZE, PACK-TENSION, STRUCT-BASE, STRUCT-SIDE, STRUCT-HEIGH, S-ENHANCE-F, S-RENEWAL-F	sectionid	—
TRAY-RATE2	AREA-FACTOR, MOLE-VHLDP, MASS-VHLDP, VOL-VHLDP, MOLE-LHLDP, MASS-LHLDP, VOL-LHLDP, VHLDP-FACTOR, LHLDP-FACTOR, BASE-STAGE, BASE-FLOOD, HOLE-PITCH	sectionid	—
MTRFC-INT, MTRFC-REAL, HTRFC-INT, HTRFC-REAL, INTFA-INT, INTFA-REAL, HOLDUP-INT, HOLDUP-REAL, USERK-INT, USERK-REAL	VALUE-LIST	—	†

† Position of a value in the INT or REAL value-list.

Block Results

Description	Sentence	Variable†	ID1	ID2
Calculated interfacial temperature	PROFRATE	TINTF	stage	—
Temperature of bulk vapor	PROFRATE	TVAP	stage	—
Calculated heat transfer rate	PROFRATE	HFLUX	stage	—
Calculated interfacial area	PROFRATE	INTF-AREA	stage	—
Calculated interfacial liquid mole composition	XY-RATE	XINTF	cid	stage
Calculated interfacial vapor mole composition	XY-RATE	YINTF	cid	stage
Calculated material mole transfer rate	XY-RATE	FLUX	cid	stage
Calculated material mole transfer rate in bulk liquid	XY-RATE	FLUXLB	cid	stage
Calculated material mole transfer rate in bulk vapor	XY-RATE	FLUXVB	cid	stage
Calculated liquid phase mole reaction rate	XY-RATE	CRATEL	cid	stage
Calculated vapor phase mole reaction rate	XY-RATE	CRATEV	cid	stage
Calculated pressure drop	PROF-RATE2	DP-STG	stage	—

† You can also access variables using the VECTOR-DEF sentence. See Chapter 29.

18 Liquid-Liquid Extraction

This chapter describes the input language for the liquid-liquid extraction model. The model is:

Model	Description	Purpose	Use
EXTRACT	Liquid-liquid extractor	Rigorous rating calculations for liquid-liquid extraction	Countercurrent liquid-liquid extractors with a feed stream to the top and bottom stage, and a product stream for the top and bottom stage. Additional side feeds, products, and heaters are allowed.

EXTRACT: Liquid-Liquid Extractor

Input Language for EXTRACT

```
BLOCK    blockid    EXTRACT
PARAM    keyword=value
```

Keyword:

NSTAGE

Optional keywords:

MAXOL MAXIL TOLOL RMSOL1 OLMETH ILMETH QMINBWOL QMAXBWOL QMINBWIL QMAXBWIL MAXIP TOLIL0 TOLILFAC TOLILMIN FMINFAC LLRATIO-REP

```
FEEDS    sid    stage  / ...
PRODUCTS    sid    stage    [phase]    [mole-flow]  / ...
PSEUDO-STREAM    sid    stage    phase    [MOLE-FLOW=value]  / ...
P-SPEC    stage    pres  / ...
HEATERS    stage    duty  / ...
T-SPEC    stage    temp  / ...
L1-COMPS    cid-list
L2-COMPS    cid-list
T-EST    stage    temp  / ...
X1-EST    stage    cid    frac  / ...
X2-EST    stage    cid    frac  / ...
COMP-EFF    stage    cid    eff  / ...
STAGE-EFF    stage    eff  / ...
basis-KLL    KLL-CID=cid    KLL-A=value    [KLL-B=value]    [KLL-C=value]    [KLL-
      D=value]
DIAGNOSTICS    keyword=value
```

Keywords:

MAIN TERM

```
REPORT    reportopt-list
```

Special reportopts:

NOPROFILE NOCOMPS NOENTH

```
TRAY-REPORT    keyword=value
```

Keywords:

TRAY-OPTION FORMAT ORDER PROPERTIES WIDE

```
INCL-TRAYS    [stage1]    [stage2]  / ...
```

PLOT **plotno** **plot-list** **comp-plot=groupid-list** *keyword=value*

Plot-list options:

TEMP **PRES** **LRATE** **LL-RATIO**

Comp-plot options:

X1 **X2** **KLL**

Optional keywords:

BASIS **ORDER** **PLOT-HEADING** **WIDE**

SUBROUTINE **KLL=subrname**
USER-VECS *keyword=value*

Keywords:

NINT **NREAL**

INT **VALUE-LIST=values**
REAL **VALUE-LIST=values**

Input Language Description for EXTRACT

PARAM Use to enter the number of stages and optional convergence parameters.

NSTAGE ..... Number of stages

MAXOL ..... Maximum number of outside loop iterations (Default=25)

MAXIL ..... Maximum number of inside loop iterations per outside loop (Default=10)

TOLOL ..... Outside loop convergence tolerance (Default=$1x10^{-4}$)

RMSOL1 ..... Threshold value of outside loop RMS error. Below this threshold EXTRACT uses the Broyden method for selected variables. (Default=0.1)

OLMETH ..... Outside loop convergence methods:

OLMETH=BROYDEN	Broyden quasi-Newton method (Default)
OLMETH=WEGSTEIN	Bounded Wegstein method

ILMETH ..... Outside loop convergence methods:

ILMETH=BROYDEN	Broyden quasi-Newton method
ILMETH=WEGSTEIN	Bounded Wegstein method
ILMETH=COMBINED	Combination of Broyden and Wegstein method (Default)

QMINBWOL ..... Minimum value of bounded Wegstein acceleration parameter for outside loop (Default=0.0)

QMAXBWOL ..... Maximum value of bounded Wegstein acceleration parameter for outside loop (Default=0.5)

QMINBWIL ..... Minimum value of bounded Wegstein acceleration parameter for inside loop (Default=0.0)

QMAXBWIL ..... Maximum value of bounded Wegstein acceleration parameter for inside loop (Default=0.5)

MAXIP ..... Maximum number of initialization calculation passes (Default=3)

TOLIL0 ..... Initial value of inside loop tolerance (Default=0.01)

TOLILFAC..... Ratio of inside loop tolerance to outside loop RMS error (Default=0.03)

TOLILMIN ..... Minimum value of inside loop tolerance (Default=$3x10^{-6}$)

FMINFAC..... Minimum allowed value for stage flow as a fraction of the total feed (Default=$1x10^{-4}$)

LLRATIO-REP ..... Whether to report the flow ratio profile of second-liquid to first-liquid:

LLARTIO-REP=YES	Include flow ratio profile in block report
LLRATIO-REP=NO	Do not include flow ratio profile in block report (Default)

FEEDS

Use to enter inlet material and heat stream stage numbers. An L1-rich stream must enter stage1. An L2-rich stream must enter NSTAGE.

sid..... Stream ID

stage..... Stage number

PRODUCTS

Use to enter outlet material and heat stream stage numbers and phases. An L1 phase stream must leave stage NSTAGE. An L2 phase stream must leave stage1. EXTRACT calculates flow rates of these streams. For all other outlet material streams, you must also specify the mole flow rate. For outlet heat streams, specify only the stream ID and stage number.

sid..... Stream ID

stage..... Stage number

phase..... **L1** First-liquid phase

L2 Second-liquid phase

mole-flow ..... Molar flow rate

PSEUDO-STREAM

Use to identify outlet streams as pseudoproduct streams and to specify the location, phase, and flow rate of the pseudoproduct stream. If you do not specify a flow rate, EXTRACT uses the net flow rate of the stage and phase (excluding any flow rate withdrawn as product).

sid..... Stream ID

stage..... Stage number

phase..... **L1** First-liquid phase

L2 Second-liquid phase

MOLE-FLOW ..... Molar flow rate

P-SPEC

Use to specify the column pressure profile.

stage..... Stage number

pres ..... Pressure

HEATERS

Use to specify heater/cooler stage locations and duties. Do not use HEATERS if you used T-SPEC. If you do not enter HEATERS or T-SPEC, the column will operate adiabatically.

stage..... Stage number

duty ..... Heat duty

T-SPEC

Use to specify a column temperature profile. These values are the final stage temperatures. EXTRACT does not adjust them. If you entered HEATERS, you cannot use T-SPEC.

stage..... Stage number

temp ..... Temperature

L1-COMPS

Use to enter a list of key components that identify the L1 phase. The liquid phase with the larger mole fraction of these key components is designated as the L1 phase.

cid-list ..... Key component ID list

L2-COMPS

Use to enter a list of key components that identify the L2 phase. The liquid phase with the larger mole fraction of these key components is designated as the L2 phase.

cid-list ..... Key component ID list

T-EST

Use to enter initial temperature profile estimates. EXTRACT adjusts these values to satisfy the stage enthalpy balances. If you do not use the T-SPEC statement, T-EST is required.

stage..... Stage number

temp ..... Temperature

X1-EST, X2-EST

Use to enter initial composition profile estimates. If you do not enter X1-EST or X2-EST, EXTRACT generates an initial profile using a built-in procedure.

stage..... Stage number

cid..... Component ID

frac ..... Liquid mole fractions of the corresponding phase

COMP-EFF

Use to enter values for separation efficiency by component. Efficiency is defined by $x_i^{L2} = (eff_i)K_i x_i^{L1}$.

Where:

K = Component distribution coefficient

x = Liquid mole fraction

i = Component index

$L1$ = Liquid phase 1

$L2$ = Liquid phase 2

You cannot use COMP-EFF, if you used STAGE-EFF.

stage..... Stage number

cid..... Component ID

eff ..... Efficiency

STAGE-EFF

Use to enter values for separation efficiency by stage. The stage efficiency is the efficiency for all components on that stage. See COMP-EFF for a definition. You cannot use STAGE-EFF, if you used COMP-EFF.

stage..... Stage number

eff ..... Efficiency

basis-KLL

Use to enter coefficients for built-in KLL expression for calculating liquid-liquid equilibrium K-values. You can enter basis-KLL in MOLE, MASS, or STDVOL basis.

KLL-CID ..... Component ID

KLL-A, KLL-B, KLL-C, KLL-D ..... Coefficients for KLL expression, which is defined as:
$\ln(KLL) = (KLL\text{-}A) + (KLL\text{-}B)/T + (KLL\text{-}C) \times \ln(T) + (KLL\text{-}D) \times T$

Where:
K = Liquid-liquid equilibrium K-value
T = Temperature in Kelvin

You must specify the value of coefficient KLL-A. Default value of the remaining coefficients is 0.0.

DIAGNOSTICS Use to enter diagnostic messages levels of convergence and simulation problems in the history and log files. The level is defined from 0 to 10. The amount of information listed increases with each level.

MAIN ..... Controls printouts of initial/final profiles, inside/outside loop iterations, and outside loop variables/functions in the history file (Default=4)

TERM ..... Controls printouts of inside and outside loop iterations in the log file (Default=0)

REPORT Use to override the default report options. You can use the standard REPORT options for use within a block (see Chapter 11) for EXTRACT.

reportopt ..... Standard block report options (see Chapter 11), in addition to the following:

NOPROFILE	Suppresses stagewise profiles of temperature, operating pressure, flows, enthalpies, and duties for this block
NOCOMPS	Suppresses mole fraction and K-value profiles for this block
NOENTH	Suppresses the enthalpy profile for this block

TRAY-REPORT Use to specify the report format and additional tray properties to be reported (in addition to the flows, temperatures, pressures, enthalpies, duties, mole fractions, and K-values printed in the standard report).

TRAY-OPTION ..... Specifies the stages included in the report:

	TRAY-OPTION=BRIEF	Reports stages that have feeds, products, heaters, maximum and minimum flows, and the stages immediately above and below those stages (Default)
	TRAY-OPTION=INCL-TRAYS	Reports the stages specified in the INCL-TRAYS statement
	TRAY-OPTION=ALL-TRAYS	Reports all stages
FORMAT	**FORMAT=PROFILE**	Prints tabular column profiles (Default)
	FORMAT=STAGE	Prints individual stage reports
	FORMAT=COMBINED	Prints both tabular column profiles and individual stage reports
ORDER	Tray numbering order. Use for report only.	
	ORDER=TOP-DOWN	Numbers stages from L1 feed down (Default)
	ORDER=BOTTOM-UP	Numbers stages from L2 feed up
PROPERTIES	List of property set IDs	
WIDE	Report width option	
	WIDE=YES	Produces wide (132 columns) reports (Default)
	WIDE=NO	Produces standard (80 columns) reports

INCL-TRAYS Use to designate stages to be included in the report when TRAY-OPTION=INCL-TRAYS in the TRAY-REPORT statement.

stage1	Stage number of initial stage of column segment to be reported
stage2	Stage number of final stage of column segment to be reported (Default=*stage1*)

PLOT Use to generate stagewise plots of column profiles. You can report properties on a MOLE, MASS, or STDVOL basis.

plotno	Plot number	
plot-list	List of non-component-dependent properties to be plotted:	
	TEMP	Temperature
	PRES	Pressure
	LRATE	Liquid flow rate of both liquids
	LL-RATIO	Second-liquid flow rate/first-liquid flow rate
comp-plot	Keyword for component-dependent property to be plotted:	
	X1, X2	Fractions of the components and/or component groups listed are plotted.
	KLL	K-values of the components and/or component groups listed are plotted. KLL is the ratio x_2/x_1
groupid-list	List of component IDs and/or component group IDs	
BASIS	**BASIS=MOLE**	Plotted results are on a mole basis (Default)
	BASIS=MASS	Plotted results are on a mass basis
	BASIS=STDVOL	Plotted results are on a standard-liquid- volume basis
ORDER	**ORDER=TOP-DOWN**	Numbers stages from top down (Default)
	ORDER=BOTTOM-UP	Numbers stages from bottom up
PLOT-HEADING	Heading up to 64 characters enclosed in quotes, printed at the top of the print-plot	
WIDE	Plot width option. Use to override default established by the PLOT-OPTIONS paragraph (See Chapter 46).	

SUBROUTINE Use to specify user-supplied KLL subroutine. For details on writing user-supplied KLL subroutine, see *Aspen Plus User Models*, Chapter 16.

KLL	User-supplied FORTRAN subroutine name for KLL calculations

USER-VECS Use to define the length of the arrays for user-supplied KLL subroutine.

NINT	Length of integer parameter array
NREAL	Length of real parameter array

INT Use to enter values for the integer parameter array of the user-supplied KLL subroutine.

VALUE-LIST	List of integer values

REAL Use to enter values for the real parameter array for the user-supplied KLL subroutine.

VALUE-LIST	List of real values

Accessing Variables in EXTRACT

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	ID2	Element
PARAM	NSTAGE	—	—	—
FEEDS	STAGE	sid	—	—
PRODUCTS	STAGE, MOLE-FLOW	sid	—	—
PSEUDO-STREAM	STAGE, MOLE-FLOW	sid	—	—
P-SPEC	PRES	stage	—	—
HEATERS	DUTY	stage	—	—
T-SPEC	TEMP	stage	—	—
T-EST	TEMP	stage	—	—
X1-EST	X1	stage	cid	—
X2-EST	X2	stage	cid	—
COMP-EFF	EFF	stage	cid	—
STAGE-EFF	EFF	stage	—	—
basis-KLL	KLL-A, KLL-B, KLL-C, KLL-D	cid	—	—
INT	VALUE	—	—	†
REAL	VALUE	—	—	†

† Position of a value in the INT or REAL value-list.

Block Results

Description	Sentence	Variable†	ID1	ID2
Stage temperature	PROFILE	TEMP	stage	—
Stage pressure	PROFILE	PRES	stage	—
Stage L1 rate	PROFILE	L1RATE	stage	—
Stage L2 rate	PROFILE	L2RATE	stage	—
Stage heat duty	PROFILE	DUTY	stage	—
L1 compositions	COMPS	X1	cid	stage
L2 compositions	COMPS	X2	cid	stage

† You can also access variables using the VECTOR-DEF sentence. See Chapter 29.

19 Reactors

This chapter describes the input language for the reactor models. The models are:

Model	Description	Purpose	Use
RSTOIC	Stoichiometric reactor	Stoichiometric reactor with specified reaction extent or conversion	When reaction kinetics are unknown or unimportant but stoichiometry and extent of reaction are known
RYIELD	Yield reactor	Reactor with specified yield	When stoichiometry and kinetics are unknown or unimportant but a yield distribution is known
REQUIL	Equilibrium reactor	Chemical and phase equilibrium by stoichiometric calculations	One- or two-phase chemical equilibrium and simultaneous phase equilibrium
RGIBBS	Equilibrium reactor (Gibbs energy minimization)	Chemical and phase equilibrium by Gibbs energy minimization	Chemical equilibrium. Simultaneous phase and chemical equilibrium. Phase equilibrium without chemical reactions. Phase equilibrium for vapor-liquid-solid systems and solid solutions.
RCSTR	Continuous stirred tank reactor	Continuous stirred tank reactor	Stirred tank reactors for vapor-liquid-solid systems with rate controlled and equilibrium reactions in any phase. Reaction kinetics are known.
RPLUG	Plug flow reactor	Plug flow reactor	Plug flow reactors for vapor-liquid-solid systems with rate controlled reactions in any phase. Reaction kinetics are known.
RBATCH	Batch reactor	Batch or semi-batch reactor	Batch and semi-batch reactors for vapor-liquid-solid systems with rate controlled reactions in any phase. Reaction kinetics are known.

RSTOIC: Stoichiometric Reactor

Input Language for RSTOIC

```
BLOCK    blockid    RSTOIC
PARAM    keyword=value
```

Keywords:

TEMP PRES VFRAC DUTY HEAT-OF-REAC

Optional keywords:

NPHASE PHASE SERIES MAXIT TOL T-EST P-EST

```
STOIC    reacno    ssid    cid    coef / [ssid]    cid    coef / . . .
EXTENT    reacno    extent / . . .
CONV    reacno    ssid    key-cid    conv / . . .
COMP-ATTR    entryno    ssid    cid    cattrname    (value-list)
SUBS-ATTR    entryno    ssid    psdid    (value-list)
SELECTIVITY    entryno    cid    ssid    ref-cid    ref-ssid / . . .
HEAT-RXN    reacno    cid    temp    pres    phase    h-reac
UTILITY    UTILITY-ID=utilityid
```

Input Language Description for RSTOIC

PARAM

Use to specify outlet conditions and whether the reactions occur simultaneously or in series. For a two-phase or three-phase flash calculation, you must specify two of the following variables: temperature, pressure, vapor fraction, or heat duty. RSTOIC accepts any combination except vapor fraction and heat duty. For a one-phase calculation, you must specify either temperature and pressure, or pressure and heat duty.

TEMP		Temperature
PRES	**PRES > 0**	Pressure
	PRES ≤ 0	Pressure drop
VFRAC		Molar vapor fraction of fluid phases. Enter 0.0 for bubble point, 1.0 for dew point. For subcooled liquid or superheated vapor, use TEMP and PRES specifications. VFRAC is allowed only when NPHASE > 1.
DUTY		Heat duty
HEAT-OF-REAC	**HEAT-OF-REAC=NO**	Does not calculate heat of reaction, nor use the specified heat of reaction in energy balances (Default)
	HEAT-OF-REAC=YES	Calculates heat of reaction, or uses the specified heat of reaction in energy balances
NPHASE		Number of phases in MIXED substream:
	NPHASE = 1	One-phase calculation
	NPHASE = 2	Two-phase flash (Default)
	NPHASE = 3	Three-phase flash
PHASE		Specifies the phase when NPHASE=1:
	PHASE = V	Vapor (Default)
	PHASE = L	Liquid
	PHASE = S	Solid. Use for electrolytes system only.
SERIES	**SERIES = NO**	Simultaneous reactions (Default)

SERIES = YES Series reactions

MAXIT ..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

TOL ..... Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

T-EST ..... Temperature estimate. Use to aid convergence when PRES and either DUTY or VFRAC are specified.

P-EST ..... Pressure estimate. Use to aid convergence when TEMP and either DUTY or VFRAC are specified.

STOIC

Use to enter the reaction stoichiometry. Enter one STOIC statement for each reaction. When SERIES=YES, *reacno* specifies the series order. For each reaction specify either the fractional conversion of a key component or the reaction extent.

reacno ..... Reaction number

ssid ..... Substream ID (Default=previous *ssid* entry)

cid ..... Component ID

coef ..... Stoichiometric coefficient (positive for products; negative for reactants). For nonconventional components, the coefficient is the mass of the component reacted or generated rather than the moles.

EXTENT

Use to specify the reaction extent, which is defined as the number of moles (mass for nonconventional components) generated for any component divided by the stoichiometric coefficient.

reacno ..... Reaction number

extent ..... Reaction extent

CONV

Use to specify the key component and its fractional conversion. The key component must be a reactant. A given component can be a key for more than one reaction. For simultaneous reactions, fractional conversion refers to the feed and does not include the reactant generated by the reactions.

reacno ..... Reaction number

ssid ..... Substream ID

key-cid ..... Key component ID

conv ..... Fractional conversion of the key component

COMP-ATTR

Use to specify outlet stream values of component attributes created or changed by the reactions. Enter one COMP-ATTR sentence for each component attribute specified.

entryno ..... Entry number

ssid ..... Substream ID

cid ..... Component ID

cattrname ..... Component attribute name

value-list ..... List of attribute values to be entered or changed. You should insert an asterisk (*) for values not changed.

SUBS-ATTR

Use to specify outlet stream values of the particle size distribution for a substream created or changed by the reactions. Enter one SUBS-ATTR sentence for each substream specified.

entryno ..... Entry number

ssid ..... Substream ID

psdid ..... Particle size distribution ID

value-list ..... List of attribute values to be entered or changed. You should insert an asterisk (*) for values not changed.

SELECTIVITY

Use to specify parameters for selectivity calculations. You must select a component and specify a reference component. Selectivity (*S*) is defined as:

$$S = \left[\frac{\Delta P}{\Delta A}\right]_{Actual} \Big/ \left[\frac{\Delta P}{\Delta A}\right]_{Ideal}$$

Where:

ΔP = Change in moles of selected component

ΔA = Change in moles of reference component

$Actual$ = Actual change in reactor

$Ideal$ = Ideal change when there are no side reactions involving the selected component or reference component

entryno ..... Entry number

cid ..... Component ID of the selected component. The selected component must be a product of a reaction.

ssid ..... Substream ID of the selected component

ref-cid ..... Component ID of the reference component. The reference component must be a reactant of a reaction.

ref-ssid ..... Substream ID of the reference component

HEAT-RXN

Use to specify the heat of reaction for each reaction when HEAT-OF-REAC=YES. You must specify a reference component for each reaction. If you do not enter h-reac, Aspen Plus calculates the heat of reaction for each reaction. If the specified heat of reaction is different from the value calculated from component heats of formation at reference conditions, Aspen Plus adjusts the block duty to match the specified heat of reaction.

reacno ..... Reaction number

cid ..... Reference component

temp ..... Reference temperature (Default=25ºC)

pres ..... Reference pressure (Default=1atm)

phase ..... Reference fluid phase

PHASE=V	Vapor (Default)
PHASE=L	Liquid

h-reac ..... Heat of reaction specification. If you specify heat of reaction for one reaction, you must specify it for all reactions.

UTILITY

Use to specify an optional utility to provide heating or cooling duty.

UTILITY-ID ..... Utility ID.

Accessing Variables in RSTOIC

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	ID2	ID3	Element
PARAM	TEMP, PRES, VFRAC, DUTY, MAXIT, TOL, T-EST, P-EST	—	—	—	—
STOIC	COEF	reacno	ssid	cid	—
EXTENT	EXTENT	reacno	—	—	—
CONV	CONV	reacno	—	—	—
COMP-ATTR	VALUE	entryno	—	—	†
SUBS-ATTR	VALUE	entryno	—	—	†
HEAT-RXN	H-REAC	reacno	—	—	—

† Position of a value in the COMP-ATTR or SUBS-ATTR value-list.

Block Results

Description	Sentence	Variable	ID1
Heat duty	PARAM	QCALC	—
Net heat duty	RESULTS	NET-DUTY	—
Reaction extent	RXN-RES	EXT-CALC	reacno
Heat of reaction	RXN-RES	H-REAC-CALC	reacno
Selectivity	SELECT-RES	SELECT-CALC	entryno

RYIELD: Yield Reactor

Input Language for RYIELD

```
BLOCK    blockid    RYIELD
PARAM    keyword=value
```

Keywords:

TEMP PRES VFRAC DUTY

Optional keywords:

NPHASE PHASE MAXIT TOL T-EST P-EST

```
MOLE-YIELD    ssid    cid    yield  /  [ssid]    cid    yield  /  . . .
MASS-YIELD    ssid    cid    yield  /  [ssid]    cid    yield  /  . . .
INERTS    cid  /  . . .
COMP-ATTR    entryno    ssid    cid    cattrname    (value-list)
SUBS-ATTR    entryno    ssid    psdid    (value-list)
LUMP    lumpid    lcid    frac  /  . . .
DE-LUMP    dlup-id    lcid    frac  /  . . .
```

PETRO-CHAR *keyword=value*

Keywords:

ASSAY-ID TBP-BASIS GRAV-TYPE VISC-TYPE DATA-SOURCE GRAV MW

TBP-CURVE percent temp / ...
GRAV-CURVE dist-temp value / ...
MW-CURVE dist-temp value / ...
PROP-CURVE prop-name dist-temp value / ...
VISC-CURVE ref-temp dist-temp value / ...
SUBROUTINE *keyword=value*

Keywords:

YIELD PETRO-CHAR

USER-VECS *keyword=value*

Keywords:

NINT NREAL NIWORK NWORK NINTP NREALP NIWORKP NWORKP

PC-SUB *keyword=value*

Keywords:

NTBMAX NGRMAX NMWMAX NPMAX NPCMAX NVCMAX

INT value-list
REAL value-list
PC-INT value-list
PC-REAL value-list
UTILITY UTILITY-ID=*utilityid*

Input Language Description for RYIELD

PARAM

Use to specify outlet conditions for the reactor. For a two-phase or three-phase flash calculation, you must specify two of the following variables: temperature, pressure, vapor fraction, or heat duty. RYIELD accepts any combination except vapor fraction and heat duty. For a one-phase calculation, you must specify either temperature and pressure, or pressure and heat duty.

TEMP	Temperature	
PRES	**PRES > 0**	Pressure
	PRES ≤ 0	Pressure drop
VFRAC	Molar vapor fraction of fluid phases. Enter 0.0 for bubble point, 1.0 for dew point. For subcooled liquid or superheated vapor, use TEMP and PRES specifications. VFRAC is allowed only when NPHASE > 1.	
DUTY	Heat duty	
NPHASE	Number of phases in MIXED substream:	
	NPHASE = 1	One-phase calculation
	NPHASE = 2	Two-phase flash (Default)
	NPHASE = 3	Three-phase flash
PHASE	Specifies the phase when NPHASE=1:	

	PHASE = V	Vapor (Default)
	PHASE = L	Liquid
	PHASE = S	Solid. Use for electrolytes system only.

MAXIT ..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

TOL ..... Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

T-EST ..... Temperature estimate. Use to aid convergence when PRES and either DUTY or VFRAC are specified.

P-EST ..... Pressure estimate. Use to aid convergence when TEMP and either DUTY or VFRAC are specified.

MOLE-YIELD Use to enter mole yields. Use for conventional components only.

ssid ..... Substream ID

cid ..... Component ID

yield ..... Mole yield (per unit *mass* of total feed)

MASS-YIELD Use to enter mass yields.

ssid ..... Substream ID

cid ..... Component ID

yield ..... Mass yield (per unit *mass* of total feed)

INERTS Use to specify the component IDs of species that do not participate in the reaction. If you specify INERTS, the total feed minus total mass of inerts is the basis for the yield calculation.

cid ..... Component ID

COMP-ATTR Use to specify outlet stream values of component attributes created or changed by the reactions. Enter one COMP-ATTR sentence for each component attribute specified.

entryno ..... Entry number

ssid ..... Substream ID

cid ..... Component ID

cattrname ..... Component attribute name

value-list ..... List of attribute values to be entered or changed. You should insert an asterisk (*) for values not changed.

SUBS-ATTR Use to specify outlet stream values of the particle size distribution for a substream created or changed by the reactions. Enter one SUBS-ATTR sentence for each substream specified.

entryno ..... Entry number

ssid ..... Substream ID

psdid ..... Particle size distribution ID

value-list ..... List of attribute values to be entered or changed. You should insert an asterisk (*) for values not changed.

LUMP Use to specify component lumping from LCID to LUMPID.

lumpid ..... Target component name in component mapping

lcid ..... Source component name in component mapping

frac ..... Coefficient for the component

DE-LUMP Use to specify component de-lumping from DLUP-ID to LCID.

dlup-id ..... Source component name in component mapping

lcid..... Target component name in component mapping

frac ..... Coefficient for the component

PETRO-CHAR Use to specify parameters for petroleum characterization.

ASSAY-ID..... Assay name

TBP-BASIS ..... TBP curve type. Also applies to TBP curve returned from user-supplied petroleum characterization routine.

TBP-BASIS = STDVOL	Standard liquid volume. (Default)
TBP-BASIS = MASS	Weight.

GRAV-TYPE ..... Gravity type for bulk gravity and gravity curve. Also applies to values returned from user-supplied petroleum characterization routine.

GRAV-TYPE = SG	Specific gravity. (Default)
GRAV-TYPE = API	American Petroleum Institute (API) gravity.

VISC-TYPE ..... Viscosity type

VISC-TYPE = DYNAMIC	Absolute viscosity (Default)
VISC-TYPE = KINEMATIC	Kinematic viscosity

DATA-SOURCE..... Data source of petroleum characterization specifications

DATA-SOURCE = INPUT	Through specified parameters and curves (Default).
DATA-SOURCE = USER	Through user-supplied Fortran routine for petroleum characterization

GRAV ..... Bulk gravity

MW ..... Bulk molecular weight

TBP-CURVE Use to enter the distillation temperature curve.

percent ..... Percent distilled. Minimum of 4 points are required for curve and all values must be in ascending order.

temp ..... Distillation temperature. Minimum of 4 points are required for curve and all values must be in ascending order. If 100% point is not given, temperature will be extrapolated to 100%.

GRAV-CURVE Use to enter the gravity curve.

dist-temp ..... Distillation temperature. Minimum of 4 points are required for curve and all values must be in ascending order.

value..... Value for gravity

MW-CURVE Use to enter the molecular weight curve.

dist-temp ..... Distillation temperature. Minimum of 4 points are required for curve and all values must be in ascending order.

value..... Value for molecular weight

PROP-CURVE Use to enter the petroleum property curve.

prop-name ..... Property name

dist-temp ..... Distillation temperature. Minimum of 4 points are required for curve and all values must be in ascending order.

	value	Value for petroleum property
VISC-CURVE	Use to enter the viscosity curve.	
	ref-temp	Reference temperature
	dist-temp	Distillation temperature. Minimum of 4 points are required for curve and all values must be in ascending order.
	value	Value for viscosity
SUBROUTINE	Use to specify user-supplied FORTRAN yield subroutine. For details on writing the RYIELD user subroutines, see *Aspen Plus User Models*, Chapter 15.	
	YIELD	User-supplied FORTRAN yield subroutine name
	PETRO-CHAR	User-supplied FORTRAN petroleum characterization subroutine name
USER-VECS	Use to define the length of arrays for the user-supplied yield and petroleum characterization subroutines.	
	NINT	Length of integer parameter array for yield subroutine
	NREAL	Length of real parameter array for yield subroutine
	NIWORK	Length of integer workspace array for yield subroutine
	NWORK	Length of real workspace array for yield subroutine
	NINTP	Length of integer parameter array for petroleum characterization subroutine
	NREALP	Length of real parameter array for petroleum characterization subroutine
	NIWORKP	Length of integer workspace array for petroleum characterization subroutine
	NWORKP	Length of real workspace array for petroleum characterization subroutine
PC-SUB	Use to define the length of arrays for the user-supplied petroleum characterization subroutine.	
	NTBMAX	Maximum number of data points allowed for TBP curves returned from user-supplied petroleum characterization routine (Default=20).
	NGRMAX	Maximum number of data points allowed for gravity curves returned from user-supplied petroleum characterization routine (Default=20).
	NMWMAX	Maximum number of data points allowed for molecular weight curves returned from user-supplied petroleum characterization routine (Default=20).
	NPMAX	Maximum number of data points allowed for petroleum property curves returned from user-supplied petroleum characterization routine. Also applies to viscosity curves (Default=20).
	NPCMAX	Maximum number of property curves allowed for user-supplied petroleum characterization routine (Default=10).
	NVCMAX	Maximum number of viscosity curves allowed for user-supplied petroleum characterization routine (Default=10).
INT	Use to enter values for the integer parameter array of the user-supplied yield subroutine.	

value-list ..... List of integer values

REAL Use to enter values for the real parameter array of the user-supplied yield subroutine.

value-list ..... List of real values

PC-INT Use to enter values for the integer parameter array of the user-supplied petroleum characterization subroutine.

value-list ..... List of integer values

PC-REAL Use to enter values for the real parameter array of the user-supplied petroleum characterization subroutine.

value-list ..... List of real values

UTILITY Use to specify an optional utility to provide heating or cooling duty.

UTILITY-ID ..... Utility ID.

Accessing Variables in RYIELD

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	ID2	Element
PARAM	TEMP, PRES, VFRAC, DUTY, MAXIT, TOL, T-EST, P-EST	—	—	—
MOLE-YIELD	YIELD	ssid	cid	—
MASS-YIELD	YIELD	ssid	cid	—
COMP-ATTR	VALUE	entryno	—	—
SUBS-ATTR	VALUE	entryno	—	—
LUMP	FRAC	lumpid	lcid	—
DE-LUMP	FRAC	dlup-id	lcid	—
PETRO-CHAR	GRAV, MW	—	—	—
INT	VALUE-LIST	—	—	†
REAL	VALUE-LIST	—	—	†
PC-INT	VALUE-LIST	—	—	†
PC-REAL	VALUE-LIST	—	—	†

† Position of a value in the INT, REAL, PC-INT, or PC-REAL value-list.

Block Results

Description	Sentence	Variable
Heat duty	PARAM	QCALC
Net heat duty	PARAM	NET-DUTY

REQUIL: Equilibrium Reactor

Input Language for REQUIL

```
BLOCK    blockid    REQUIL
PARAM    keyword=value
```

Keywords:

NREAC TEMP PRES VFRAC DUTY

Optional keywords:

NPHASE PHASE ENTRN CHEM-MAXIT CHEM-TOL MAXIT TOL T-EST P-EST

```
STOIC    reacno    cid    coef    phase  /  cid    coef    phase  /  . . .
EXTENT-SPEC    reacno    extent  /  . . .
EXTENT-EST    reacno    extent  /  . . .
TAPP-SPEC    reacno    delt  /  . . .
FRAC    ssid    vapor  /  . . .
UTILITY    UTILITY-ID=utilityid
```

Input Language Description for REQUIL

PARAM

Use to specify outlet conditions for the reactor and optional convergence parameters. For a two-phase flash calculation, you must specify two of the following variables: temperature, pressure, vapor fraction, or heat duty. REQUIL accepts any combination, except vapor fraction and heat duty. For a one-phase calculation, you must specify either temperature and pressure, or pressure and heat duty. REQUIL cannot perform three-phase calculations.

NREAC	Number of reactions	
TEMP	Temperature	
PRES	**PRES > 0**	Pressure
	PRES ≤ 0	Pressure drop
VFRAC	Molar vapor fraction of fluid phases. Enter 0.0 for bubble point, 1.0 for dew point. For subcooled liquid or superheated vapor, use TEMP and PRES specifications. VFRAC is allowed only when NPHASE > 1.	
DUTY	Heat duty	
NPHASE	Number of phases in MIXED substream:	
	NPHASE = 1	One-phase calculation
	NPHASE = 2	Two-phase flash (Default)
PHASE	Specifies the phase when NPHASE=1:	
	PHASE = V	Vapor (Default)
	PHASE = L	Liquid
	PHASE = S	Solid. Use for electrolytes system only.
ENTRN	Fraction of the liquid phase that is entrained in the vapor stream. (Default=0)	
CHEM-MAXIT	Maximum number of iterations for chemical equilibrium calculations. The REQUIL algorithm performs flash calculations nested inside a chemical equilibrium loop. (Default=30)	

CHEM-TOL ..... Tolerance for chemical equilibrium calculations. (Default=$2x10^{-5}$)

MAXIT ..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

TOL ..... Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

T-EST ..... Temperature estimate. Use to aid convergence when PRES and either DUTY or VFRAC are specified.

P-EST ..... Pressure estimate. Use to aid convergence when TEMP and either DUTY or VFRAC are specified.

STOIC Use to enter the reaction stoichiometry. Enter one STOIC statement for each reaction. The reactions must be linearly independent.

reacno ..... Reaction number

cid ..... Component ID (conventional component only)

coef ..... Stoichiometric coefficient (positive for products; negative for reactants)

phase ..... ***** Component is not a solid

S Component is a solid

EXTENT-SPEC Use to fix the molar extent of a reaction, defined as the number of moles generated for any component divided by the stoichiometric coefficient. Do not enter EXTENT-SPEC for a reaction that has a temperature approach specified by TAPP-SPEC.

reacno ..... Reaction number

extent ..... Fixed molar extent of reaction, defined as moles generated for any component divided by the stoichiometric coefficient

EXTENT-EST Use to provide an optional initial estimate for reaction extents that are not fixed by EXTENT-SPEC.

reacno ..... Reaction number

extent ..... Estimate for molar extent of reaction, defined as moles generated for any component divided by the stoichiometric coefficient

TAPP-SPEC Use to specify a temperature approach to chemical equilibrium for a reaction. The computed chemical equilibrium constant for the reaction is evaluated at the temperature $T + \Delta T$ where T is the actual reactor temperature and ΔT is the temperature approach. If you want a temperature approach for the entire system, you must specify it for each reaction. You cannot use TAPP-SPEC for a reaction with an EXTENT-SPEC.

reacno ..... Reaction number

delt ..... Number of degrees above the system temperature at which Aspen Plus calculates the chemical equilibrium for this reaction

FRAC Use to specify solids entrainment in the vapor stream. Any remaining solids are placed in the liquid outlet stream.

ssid ..... Solids substream ID

vapor ..... Fraction of total solids (after reaction) in the specified substreams that is placed in the corresponding substream of vapor outlet stream. (Default=0)

UTILITY Use to specify an optional utility to provide heating or cooling duty.

UTILITY-ID ..... Utility ID.

Accessing Variables in REQUIL

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	ID2
PARAM	TEMP, PRES, VFRAC, DUTY, ENTRN, CHEM-MAXIT, CHEM-TOL, MAXIT, TOL, T-EST, P-EST	—	—
STOIC	COEF, PHASE	reacno	cid
EXTENT-SPEC	EXTENT	reacno	—
EXTENT-EST	EXTENT	reacno	—
TAPP-SPEC	DELT	reacno	—
FRAC	VAPOR	ssid	—

Block Results

Description	Sentence	Variable	ID1
Heat duty	RESULTS	QCALC	—
Net heat duty	RESULTS	NET-DUTY	—
Equilibrium constant	RXN-RES	K-CALC	reacno

RGIBBS: Equilibrium Reactor - Gibbs Energy Minimization

Input Language for RGIBBS

```
BLOCK    blockid    RGIBBS
PARAM    keyword=value
```

Keywords:

TEMP PRES DUTY

Optional keywords:

NPHASE VAPOR CHEMEQ NATOM NREAC TAPP MAXIT TOL SOLIDS TEST TUPPER TLOWER EB-MAXIT EB-TOL NPSOL

```
PROD    cid    [ phase]    [flow-est]  /  . . .
PROD-MOLES    cid    flow  /  . . .
PROD-FRAC    cid    frac  /  . . .
MOLE-FLOWEST flowcid flowest / . . .
PHASES    phaseid    phase    COMPS=comp-list
PHASE-PROPERTY    phaseid    propname
STOIC    reacno    cid    coef  /  cid    coef  /  . . .
EXTENT-SPEC    reacno    extent  /  . . .
TAPP-SPEC    reacno    delt  /  . . .
```

```
KEY    sid    cutoff    cid-list / . . .
ATOM cid        1        coef1  / coef2 / . . . / coefNATOM /
        .
        .
        .
      cid       1        coef1 / coef2 / . . . / coefNATOM
UTILITY    UTILITY-ID=utilityid
```

Input Language Description for RGIBBS

PARAM

Use to specify outlet conditions of the reactor and parameters that control the calculations. You must specify either temperature and pressure, or pressure and heat duty. By default, vapor phase chemical equilibrium is considered.

TEMP	Temperature	
PRES	**PRES > 0**	Pressure
	PRES ≤ 0	Pressure drop
DUTY	Heat duty	
NPHASE	Maximum number of fluid phases considered	
VAPOR	**VAPOR = NO**	Does not consider a vapor phase
	VAPOR = YES	Considers a vapor phase (Default)
CHEMEQ	**CHEMEQ = NO**	Does not calculate chemical equilibrium
	CHEMEQ = YES	Calculates chemical equilibrium (or restricted chemical equilibrium) (Default)
NATOM	Number of atoms present in the system. Use only when CHEMEQ=YES and ATOM is entered.	
NREAC	Number of chemical reactions. Use only for restricted equilibrium calculations involving individual reactions. You must give NREAC when the STOIC statement is used.	
TAPP	Temperature approach for the entire system, defined as the number of degrees above the reactor temperature at which the chemical equilibrium is computed. Use TAPP only when CHEMEQ=YES. If you want a temperature approach for an individual reaction, use the TAPP-SPEC statement instead of TAPP. (Default=0)	
MAXIT	Maximum number of iterations (Default=50)	
TOL	Convergence tolerance (Default=1×10^{-4})	
SOLIDS	Stream ID for stream in which all solid products are placed (Default=last outlet stream)	
TEST	Temperature estimate. Used to aid convergence when pressure and duty are specified. (Default=feed temperature)	
TUPPER	Upper bound on temperature when DUTY is specified. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	
TLOWER	Lower bound on temperature when DUTY is specified. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	
EB-MAXIT	Maximum iterations for the energy balance calculations in the case when DUTY is specified (Default=50)	

EB-TOL..... Tolerance for the energy balance calculations in the case when DUTY is specified (Default=$1x10^{-4}$)

NPSOL..... Maximum number of solid solution phases considered (Default=0)

PROD Use to enter the list of products expected at equilibrium. Use only when chemical equilibrium is calculated (CHEMEQ=YES). You can also enter initial estimates of product flow rates.

cid..... Component ID

phase..... Phase(s) in which components can appear. (See Table 20.1.)

flow-est ..... Initial estimate of the product mole flow rate

PROD-MOLES Use to enter fixed outlet amounts for any component in the product list. It is used only when CHEMEQ=YES.

cid..... Component ID

flow ..... Component molar flow

PROD-FRAC Use to enter the fraction of a feed component that does not react. It is used only when CHEMEQ=YES.

cid..... Component ID

frac ..... Mole fraction of the feed

MOLE-FLOWEST Use to specify initial estimates for the outlet component flow rates on a mole basis. It is used only when CHEMEQ=YES.

flowcid..... Component ID

flowest..... Flow rate estimate on a mole basis

PHASES Use to define phases that can exist at equilibrium, and the components in each phase. By default, RGIBBS distributes all solution species among all solution phases. You can assign different thermodynamic option sets to each of these phases using the PHASE-PROPERTY sentence.

phaseid..... Phase ID given to identify a phase

phase..... Physical state of the phase:

V	Vapor
L	Liquid
S	Solid solution
SS	Single solid

comp-list..... List of components allowed to exist in the phase (Default=all components)

PHASE-PROPERTY Use to assign thermodynamic option sets to each phase specified in the PHASES sentence.

phaseid..... Phase ID given to identify a phase

propname ..... Name of property option set for the phase specified in PHASES sentence

STOIC Use to specify stoichiometric coefficients when an individual reaction is restricted from reaching equilibrium through an EXTENT-SPEC or TAPP-SPEC statement. You must enter a complete set of linearly independent reactions for the participating components, even if only one reaction is restricted. Enter one STOIC statement for each reaction. You must enter NREAC when the STOIC statement is used.

reacno ..... Reaction number

cid..... Component ID

coef..... Stoichiometric coefficient (positive for products; negative for reactants)

EXTENT-SPEC Use to fix the molar extent for any reaction defined by a STOIC statement. Do not enter EXTENT-SPEC for a reaction that has a temperature approach specified by TAPP-SPEC.

reacno ..... Reaction number

extent ..... Molar extent of reaction, defined as moles generated for any component divided by stoichiometric coefficient

TAPP-SPEC Use to specify a temperature approach to chemical equilibrium for any reaction defined by a STOIC statement. Do not enter a temperature approach for a reaction that has an extent fixed by an EXTENT-SPEC statement. If you want a temperature approach for the entire system, use the TAPP entry in the PARAM sentence instead of TAPP-SPEC.

reacno ..... Reaction number

delt ..... Number of degrees above the reactor temperature at which RGIBBS calculates the chemical equilibrium for this reaction (Default=0)

KEY Use to assign the phases computed by RGIBBS to the outlet streams when the block has multiple outlet material streams. A KEY statement is used to label the liquid phases computed by RGIBBS with key components. If you do not use a KEY statement and the block has more than one outlet stream, Aspen Plus uses the first outlet stream listed in the FLOWSHEET paragraph for the vapor phase (if VAPOR=YES). The remaining outlet streams are successively assigned the liquid phases computed by RGIBBS. If there are more phases than outlet streams, the extra liquid phases are blended into the last outlet stream.

sid..... Outlet stream ID

cutoff ..... Minimum mole fraction of the key components that a phase must have before it can be assigned to the given outlet stream. If *cutoff* is negative the stream is reserved for the vapor phase.

cid-list ..... List of one or more key components desired in high concentration in the given outlet stream. Do not enter this list for the vapor stream.

ATOM Use to enter the atomic formula for all feed and product components when chemical equilibrium is considered (CHEMEQ=YES) and the physical property parameter NATOM is not available for each possible feed and product component. If you enter ATOM, you must also enter NATOM in the PARAM sentence.

cid..... Component ID

coef..... Stoichiometric number of the given atom in the component. Enter 0 if the atom does not appear in the component formula. In setting up the atom matrix, the atoms are ordered arbitrarily one through NATOM. It is convenient to place a comment line (; ATOMS) above the ATOM statement, listing atoms in the chosen order.

UTILITY Use to specify an optional utility to provide heating or cooling duty.

UTILITY-ID ..... Utility ID.

Table 20.1 Phase Options

Phase	Description
M	Mixed phase (Default)
V	Vapor
L	Liquid
S	Solid solution
SS	Single solid. A solid phase containing only a single solid species.
L1	First-liquid
L2	Second-liquid
L3	Third-liquid
L4	Fourth-liquid
L5	Fifth-liquid
S1	First-solid solution
S2	Second-solid solution
VL	Vapor-liquid phase
VL1	Vapor/first-liquid phase
VL2	Vapor/second-liquid phase
VL3	Vapor/third-liquid phase
VL4	Vapor/fourth-liquid phase
VL5	Vapor/fifth-liquid phase
L1L2	First-liquid/second-liquid phase
L1L3	First-liquid/third-liquid phase
L1L4	First-liquid/fourth-liquid phase
L1L5	First-liquid/fifth-liquid phase
L2L3	Second-liquid/third-liquid phase
L2L4	Second-liquid/fourth-liquid phase
L2L5	Second-liquid/fifth-liquid phase
L3L4	Third-liquid/fourth-liquid phase
L3L5	Third-liquid/fifth-liquid phase
L4L5	Fourth-liquid/fifth-liquid phase
VL1L2	Vapor/first-liquid/second-liquid phase
VL1L3	Vapor/first-liquid/third-liquid phase
VL2L3	Vapor/second-liquid/third-liquid phase
VLS	Vapor/liquid/solid solution
VL1S	Vapor/first-liquid/solid solution
VL2S	Vapor/second-liquid/solid solution
VL3S	Vapor/third-liquid/solid solution
LS	Liquid/solid solution
L1S	First-liquid/solid solution
L2S	Second-liquid/solid solution
L3S	Third-liquid/solid solution
L1L2S	First-liquid/second-liquid/solid solution
L1L3S	First-liquid/third-liquid/solid solution
L2L3S	Second-liquid/third-liquid/solid solution

Accessing Variables in RGIBBS

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	ID2
PARAM	TEMP, PRES, DUTY, TAPP, MAXIT, TOL, TEST	—	—
PROD	FLOW-EST	cid	—
PROD-MOLES	FLOW	cid	—
PROD-FRAC	FRAC	cid	—
STOIC	COEF	reacno	cid
EXTENT-SPEC	EXTENT	reacno	—
TAPP-SPEC	DELT	reacno	—
KEY	CUTOFF	sid	—
ATOM	COEF	cid	atom1†

† Atom1 is the column number in the atom matrix.

Block Results

Description	Sentence	Variable	ID1
Vapor fraction	PARAM	VFRAC	—
Heat duty	PARAM	QCALC	—
Net heat duty	RESULTS	NET-DUTY	—
Equilibrium constant	RXN-RES	K-CALC	reacno

RCSTR: Continuous Stirred Tank Reactor

Input Language for RCSTR

```
BLOCK    blockid    RCSTR
PARAM    keyword=value
```

Keywords:

VOL RES-TIME PHASE-RES-TIME TEMP PRES DUTY

Optional keywords:

ALGORITHM NPHASE PHASE PHASE-VOL PHASE-VOL-FRAC TEST MAXIT TOL MB-MAXIT MB-TOL FLASH-MAXIT FLASH-TOL RET-THRESH TRACE MAX-IL-CUT MAX-OL-CUT IL-DAMP OL-DAMP MAX-TSTEP DAMP-FAC SCALING COMP-ATTR SUBS-ATTR MAX-NSTEP INT-TOL HINIT CORR-TOL CORR-METHOD ERR-METHOD MAX-STEPSIZE RAMP-TIME RAMPING CUTOFF NONNEG VOL-EST PHASE-VOL-EST RT-TOL RT-MAXIT MAX-VSTEP

```
REACTIONS    reacid-list
STOIC    reacno    ssid    cid    coef / [ssid]    cid    coef / . . .
RATE-CON    reacno    pre-exp    act-energy    [temp-exponent] / . . .
POWLAW-EXP    reacno    cid    exponent / . . .
L2-COMPS    keyword=value
```

Keywords:

COMP-LIST L2-CUTOFF

```
basis-FLOW    ssid    cid    flow / . . .
COMP-ATTR    entryno    ssid    cid    cattrname    (value-list)
SUBS-ATTR    entryno    ssid    psdid    (value-list)
CONVERGENCE    keyword=value
```

Keywords:

SOLVER TOL-FUNC MAX-BOUND MAX-DIVERGE JAC-METHOD DOGLEG-ITERS FLOW-LB FLOW-UB FLOW-DXUB EXTENT-LB EXTENT-UB EXTENT-DXUB STAB-STRAT

```
SUBROUTINE    KINETICS=subrname
USER-VECS    keyword=value
```

Keywords:

NINT NREAL NIWORK NWORK

```
INT    value-list
REAL    value-list
UTILITY    UTILITY-ID=utilityid
```

Input Language Description for RCSTR

PARAM

Use to specify outlet conditions for the reactor, volume, residence time, and optional convergence parameters. You must specify pressure, and either heat duty or temperature. You must also specify one of volume, residence time, and phase residence time. You can specify that one-, two-, or three-phase flash calculations be performed in the reactor. The default is to perform vapor phase calculations. To promote convergence, you can supply estimates for temperature and volume.

VOL	Reactor volume	
TEMP	Reactor temperature	
PRES	**PRES > 0**	Pressure
	PRES ≤ 0	Pressure drop
DUTY	Reactor heat duty	
ALGORITHM	Initialization algorithm for the mass balance equations:	
	ALGORITHM=SOLVER	Uses the simultaneous equation solver to solve the model equations (Default)
	ALGORITHM= INTEGRATOR	Uses the integrator to obtain a good initial guess of the steady state solution. This guess is then used by the simultaneous equation solver.
	ALGORITHM=MIXED	Use the integrator to initialize the first time only, and use the simultaneous equation solver on subsequent passes.
NPHASE	Number of phases in MIXED substream:	
	NPHASE=1	One-phase calculation (Default)
	NPHASE=2	Two-phase flash
	NPHASE=3	Three-phase flash
PHASE	When NPHASE=1, PHASE specifies the reactor phase. When NPHASE=2 or 3, PHASE identifies the phase referenced by PHASE-VOL, PHASE-VOL-FRAC, and PHASE-RES-TIME. When NPHASE=2 or 3, and the REACTIONS paragraph is not used to specify the reaction kinetics, PHASE also identifies the reacting phase.	
	PHASE=V	Vapor (Default)
	PHASE=L	Liquid
PHASE-VOL	Volume of the specified phase when NPHASE=2 or 3	
PHASE-VOL-FRAC	Volume of the specified phase, as a fraction of the reactor volume, when NPHASE=2 or 3	
TEST	Temperature estimate. Use to aid convergence when PRES and DUTY are specified. (Default=inlet temperature)	
MAXIT	Maximum number of iterations for energy balance calculations. Use only when DUTY is specified. (Default=30)	
TOL	Tolerance for energy balance calculations. Use only when DUTY is specified. (Default=$1x10^{-4}$)	
MB-MAXIT	Maximum number of iterations for mass balance calculations (Default=30)	
MB-TOL	Tolerance for mass balance calculations (Default=TOL/10)	
FLASH-MAXIT	Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	

FLASH-TOL Tolerance for flash calculations. Defaults to the smaller of MB-TOL/10 and the global flash tolerance established by the SIM-OPTIONS paragraph. (See Chapter 45.)

RET-THRESH Threshold value for error below which flash retention is used. Applies when RESTART=YES. (See Chapter 11.) (Default=$1x10^{10}$)

TRACE Scale factor threshold (Default=0.001)

MAX-IL-CUT Maximum number of consecutive mass balance loop damping steps. Allowed only when SOLVER=BROYDEN. (Default=5)

MAX-OL-CUT Maximum number of consecutive energy balance loop damping steps (Default=5)

IL-DAMP Damping factor on variables in the mass balance loop. Allowed only when SOLVER=BROYDEN. (Default=0.5)

OL-DAMP Damping factor on variables in the energy balance loop (Default=0.5)

MAX-TSTEP Maximum temperature step for the energy balance loop (Default=90ºF)

DAMP-FAC Damping factor. Use to control the step size of the convergence method. For no damping, set DAMP-FAC=1. Decreasing the DAMP-FAC will increase damping. (Default=1)

SCALING Scaling method for mass balance loop:

SCALING=COMPONENTS	Component-based scaling (Default)
SCALING=SUBSTREAMS	Substream-based scaling

COMP-ATTR Flag used to determine whether to integrate component attributes, using the user-supplied subroutine:

COMP-ATTR=YES	Integrates component attributes
COMP-ATTR=NO	Does not integrate component attributes (Default)

SUBS-ATTR Flag used to determine whether to integrate substream attributes, using the user-supplied subroutine:

SUBS-ATTR=YES	Integrates substream attributes
SUBS-ATTR=NO	Does not integrate substream attributes (Default)

MAX-NSTEP Number of integration steps allowed before integration is terminated. Allowed only when ALGORITHM=INTEGRATOR. (Default=1000)

INT-TOL Convergence tolerance for integration procedure. Allowed only when ALGORITHM=INTEGRATOR. (Default=MB-TOL)

HINIT Initial step size of the integration variable. Defined as a factor of reactor residence time. Allowed only when ALGORITHM=INTEGRATOR. (Default=$1x10^{-4}$)

CORR-TOL Ratio of the corrector tolerance to the integration tolerance. Allowed only when ALGORITHM=INTEGRATOR. (Default=0.1)

CORR-METHOD Corrector convergence method. Allowed only when ALGORITHM=INTEGRATOR.

CORR-METHOD=NEWTON	Newton method (Default)
CORR-METHOD=DIRECT	Direct substitution method

ERR-METHOD Error scaling method. Allowed only when ALGORITHM=INTEGRATOR.

ERR-METHOD=STATIC Constant scaling of error (Default)

ERR-METHOD=DYNAMIC Dynamic scaling of error

MAX-STEPSIZE Maximum step size of the integration variable, defined as a factor of reactor residence time. Allowed only when ALGORITHM=INTEGRATOR.

RAMP-TIME Ramping interval. Defined as a factor of reactor residence time. Allowed only when ALGORITHM=INTEGRATOR and RAMPING=YES. (Default=5)

RAMPING Variable ramping option: YES or NO. Allowed only when ALGORITHM=INTEGRATOR. (Default=NO)

CUTOFF Cutoff value for dependent variables below which integration error is ignored. If you specify ERR-METHOD=STATIC, the cutoff value will not have an appreciable effect on the integrator performance. Allowed only when ALGORITHM=INTEGRATOR. (Default=$1x10^{-10}$)

NONNEG Non-negativity flag: YES or NO. Use to force integration variables to have positive values. Allowed only when ALGORITHM=INTEGRATOR. (Default=NO)

RES-TIME Residence time for the reactor (composite for all phases)

PHASE-RES-TIME Residence time for the specified phase when NPHASE=2 or 3

VOL-EST Estimate for the reactor volume. Use to aid convergence when RES-TIME is specified.

PHASE-VOL-EST Estimate for the volume of the specified phase when NPHASE=2 or 3. Use to aid convergence when PHASE-RES-TIME is specified.

RT-TOL Error tolerance for the residence time convergence loop. Use when RES-TIME or PHASE-RES-TIME is specified. (Default=$1x10^{-4}$)

RT-MAXIT Maximum number of iterations for the residence time convergence loop. Use when RES-TIME or PHASE-RES-TIME is specified. (Default=50)

MAX-VSTEP Maximum volume step (as a factor of the initial volume estimate) for the residence time convergence loop. Use when RES-TIME or PHASE-RES-TIME is specified. (Default=1.0)

REACTIONS

Use to enter the IDs of the REACTIONS paragraphs that define the reactions. (See Chapter 6.) RCSTR can handle equilibrium and kinetic type reactions.

reacid-list List of reaction paragraph IDs

STOIC

Use to specify the stoichiometric coefficients for each reaction. The use of this sentence is obsolete, but is maintained here for upward compatibility. Use the REACTIONS sentence instead.

ssid Substream ID

reacno Reaction number

cid Component ID

coef Stoichiometric coefficient (positive for products; negative for reactants)

RATE-CON

Use to specify the pre-exponential factor, the temperature exponent, and the activation energy for each reaction. The use of this sentence is obsolete, but is maintained here for upward compatibility. Use the REACTIONS sentence instead.

reacno Reaction number

pre-exp ..... Pre-exponential factor. Units must be in SI. (See the *Aspen Plus User Guide*.)

act-energy ..... Activation energy. (Units keyword is MOLE-ENTHALPY.)

temp-exponent ..... Temperature exponent for temperature in Kelvin (Default=0)

POWLAW-EXP Specifies the exponents for the components participating in each reaction. If the order of the reaction with respect to a component is zero, you do not have to enter that component. The use of this sentence is obsolete, but is maintained here for upward compatibility. Use the REACTIONS sentence instead.

reacno ..... Reaction number

cid..... Component ID

exponent ..... Exponent. Need not be an integer.

L2-COMPS Use to enter a list of components that are used to identify the second-liquid phase when NPHASE=3 and FREE-WATER=NO.

COMP-LIST..... List of component IDs in the second-liquid phase

L2-CUTOFF..... Mole fraction of second phase key component above which a phase is identified as the second-liquid phase (Default=0.5)

basis-FLOW Use to specify initial estimates for the outlet component flow rates on MOLE, MASS, or STDVOL basis. Flow rate estimates can be required to aid convergence.

ssid ..... Substream ID (Default=previous *ssid* entry)

cid..... Component ID

flow ..... Flow rate estimate. Basis are MOLE and STDVOL for conventional components and MASS for nonconventional components. (Default=inlet flow rate)

COMP-ATTR Use to specify outlet stream values of component attributes created or changed by the reactions. Enter one COMP-ATTR sentence for each component attribute specified.

entryno ..... Entry number

ssid ..... Substream ID

cid..... Component ID

cattrname ..... Component attribute name

value-list ..... List of attribute values to be entered or changed. You should insert an asterisk (*) for values not changed.

SUBS-ATTR Use to specify outlet stream values of the particle-size distribution for a substream created or changed by the reactions. Enter one SUBS-ATTR sentence for each substream specified.

entryno ..... Entry number

ssid ..... Substream ID

psdid..... Particle size distribution ID

value-list ..... List of attribute values to be entered or changed. You should insert an asterisk (*) for values not changed.

CONVERGENCE Use to enter convergence parameters for solving the mass balance equations.

SOLVER..... Solution method for the mass balance equation:

SOLVER=BROYDEN	Uses the Broyden method to solve the mass balance equations (Default)

		SOLVER=NEWTON	Uses the Newton method to solve mass balance equations. Use this method if equilibrium reactions are present.
	TOL-FUNC	Function error tolerance (Default=$1x10^{-10}$)	
	MAX-BOUND	Allowed maximum number of iterations for which variables can be on bounds	
	MAX-DIVERGE.....	Allowed maximum number of iterations for which function norm diverges	
	JAC-METHOD.....	Jacobian update method:	
		JAC-METHOD=EXTERNAL	Jacobian is updated by numerical differentiation of the equations (Default)
		JAC-METHOD=SCHUBERT	Jacobian is updated by Schubert's method
	DOGLEG-ITERS	Number of initial dogleg iterations (Default=2)	
	FLOW-LB.....	Lower bound on flow variables (Default=0.0)	
	FLOW-UB	Upper bound on flow variables (Default=$1x10^{5}$)	
	FLOW-DXUB.....	Upper bound on step size of flow variables (Default =1000)	
	EXTENT-LB.....	Lower bound on reaction extent variables (Default=$-1x10^{5}$)	
	EXTENT-UB	Upper bound on reaction extent variables (Default=$1x10^{5}$)	
	EXTENT-DXUB.....	Upper bound on step size of reaction extent variables (Default =1000)	
	STAB-STRAT.....	Stabilization strategy for Newton's method	
		STAB-STRAT=DOGLEG	Dogleg strategy (Default)
		STAB-STRAT=LINE-SEARCH	Line search method
SUBROUTINE	Use to specify user-supplied kinetic subroutine. For details on writing user-supplied kinetic subroutines, see *Aspen Plus User Models*, Chapter 11. The use of this sentence is obsolete, but is maintained here for upward compatibility. Use the REACTIONS paragraph instead.		
	KINETICS.....	User-supplied FORTRAN subroutine name for kinetic calculations	
USER-VECS	Use to define the length of arrays for the user-supplied kinetic subroutine.		
	NINT.....	Length of integer parameter array	
	NREAL.....	Length of real parameter array	
	NIWORK	Length of integer workspace array	
	NWORK.....	Length of real workspace array	
INT	Use to enter values for the integer parameter array of the user-supplied kinetic subroutine.		
	value-list	List integer values	
REAL	Use to enter values for the real parameter array of the user-supplied kinetic subroutine.		
	value-list	List of real values	
UTILITY	Use to specify an optional utility to provide heating or cooling duty.		
	UTILITY-ID	Utility ID.	

Accessing Variables in RCSTR

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	ID2	ID3	Element
PARAM	VOL, TEMP, PRES, DUTY, TEST, MAXIT, TOL, MB-MAXIT, MB-TOL, PHASE-VOL, PHASE-VOL-FRAC, MAX-TSTEP, RES-TIME, PHASE-RES-TIME, VOL-EST, PHASE-VOL-EST, RT-TOL, RT-MAXIT, MAX-VSTEP	—	—	—	—
STOIC	COEF	reacno	ssid	cid	—
RATE-CON	PRE-EXP, ACT-ENERGY, TEMP-EXPONENT	reacno	—	—	—
POWLAW-EXP	EXPONENT	reacno	cid	—	—
basis-FLOW	FLOW	ssid	cid	—	—
INT	VALUE-LIST	—	—	—	=
REAL	VALUE-LIST	—	—	—	†
COMP-ATTR	VALUE	entryno	—	—	—
SUBS-ATTR	VALUE	entryno	—	—	—

† Position of a value in the INT or REAL value-list.

Block Results

Description	Sentence	Variable
Heat duty	PARAM	QCALC
Reactor temperature	PARAM	TCALC
Net heat duty	PARAM	NET-DUTY
Reactor volume	RESULTS	VOL-CALC
Volume of vapor phase in reactor	RESULTS	VOLV-CALC
Volume of liquid phase in reactor	RESULTS	VOLL-CALC
Volume of liquid 1 phase in reactor	RESULTS	VOLL1-CALC
Volume of salts in reactor	RESULTS	VOLST-CALC
Volume of condensed phases in reactor	RESULTS	VOLLS-CALC
Reactor residence time	RESULTS	RT-CALC
Residence time of vapor phase	RESULTS	RTV-CALC
Residence time of condensed phases	RESULTS	RTLS-CALC

RPLUG: Plug Flow Reactor

Input Language for RPLUG

BLOCK **blockid** **RPLUG**
PARAM *keyword=value*

Keywords:

TYPE **LENGTH** **DIAM**

Optional keywords:

NTUBE **NPHASE** **PHASE** **PRES** **PDROP** **U** **MIX** **FLASH** **UCM** **UCS** **USM** **NPOINT** **MAX-NSTEP** **HINIT** **INT-TOL** **CORR-METHOD** **CORR-TOL-RATIO** **COMP-ATTR** **SUBS-ATTR** **ERR-METHOD** **PDROP-OPTION** **EB-TOL-RATIO**

INTEG-PARAMS *keyword=value*

Keywords:

MAXSTEP **CUTOFF** **NONNEG**

COOLANT *keyword=value*

Optional keywords:

PRES **PDROP** **NPHASE** **PHASE** **TEMP** **VFRAC** **MAXIT** **TOL**

T-SPEC **loc** **temp / . . .**
REACTIONS **reacid-list**
STOIC **reacno** **ssid** **cid** **coef / cid** **coef / . . .**
RATE-CON **reacno** **pre-exp** **act-energy** **[temp-exponent]**
POWLAW-EXP **reacno** **cid** **exponent / cid** **exponent / . . .**
L2-COMPS *keyword=value*

Keywords:

COMP-LIST **L2-CUTOFF**

REGR-POINTS **setno** **profdataid** **VALUE-LIST=value-list**
REGR-PARAM **MAXPOINT=value**
PROPERTIES **opsetname** *keyword=value* **[/ opsetname** *keyword=value* **]**

Optional keywords:

FREE-WATER **SOLU-WATER** **HENRY-COMPS**

REPORT *reportopt-list*

Special reportopts:

NOPROFILE **NOCOMPS** **USERVECS**

PROP-REPORT **PROPERTIES=propsetid-list** *keyword=value*

Optional keywords:

PRINT-PLOT **Y-SCALE** **PLOT-HEADING** **WIDE** **GRID** **INTERPOLATE**

PLOT **plotno** **plot-list** **comp-plot=groupid-list** *keyword=value*

Plots:

TEMP **PRES** **VFRAC**

Optional comp-plots:

X **Y** **Z**

Optional keywords:

Y-SCALE **PLOT-HEADING** **WIDE** **GRID** **INTERPOLATE**

PLOT-COOLANT **plotno** **plot-list** **comp-plot=groupid-list** *keyword=value*

Plot:

TEMP

Optional comp-plots:

X **Y**

Optional keywords:

Y-SCALE **PLOT-HEADING** **WIDE** **GRID** **INTERPOLATE**

SUBROUTINE *keyword=value*

Keywords:

KINETICS **PRES-DROP** **QTRANS**

USER-VECS *keyword=value*

Optional keywords:

NINT **NREAL** **NIWORK** **NWORK** **NINTP** **NREALP** **NIWORKP** **NWORKP**
NINTQ **NREALQ** **NIWORKQ** **NWORKQ** **NUSER-PROF**

INT **value-list**
REAL **value-list**
INTP **value-list**
REALP **value-list**
INTQ **value-list**
REALQ **value-list**
USER-PROF **varno** *keyword=value*

Keywords:

LABEL **UNIT-LABEL**

Input Language Description for RPLUG

PARAM

Use to specify reactor dimensions, operating conditions, and optional convergence parameters. You must specify reactor length, diameter, and type. You can specify that one-, two-, or three-phase flash calculations be performed in the reactor. For two-phase calculations, you can specify whether the reactions occur in the liquid phase or the vapor phase. The default is to perform vapor phase calculations.

TYPE	**TYPE=T-SPEC**	Reactor with temperature or temperature profile specified
	TYPE=ADIABATIC	Adiabatic reactor
	TYPE=S-ADIABATIC	Adiabatic reactor. Solids can be at a different temperature than fluid phase.

	TYPE=TCOOL-SPEC	Reactor with specified coolant temperature
	TYPE=S-TCOOL-SPEC	Reactor with specified coolant temperature. Solids can be at a different temperature than fluid phase.
	TYPE=CO-COOL	Reactor with cocurrent external coolant
	TYPE=S-CO-COOL	Reactor with cocurrent external coolant. Solids can be at a different temperature than fluid phase.
	TYPE=COUNTER-COOL	Reactor with countercurrent external coolant
	TYPE=S-COUNTER-COOL	Reactor with countercurrent external coolant. Solids can be at a different temperature than fluid phase.

For types without the S prefix, any solids present are assumed to be at the same temperature as the fluid phase.

LENGTH Reactor length

DIAM Reactor diameter. If NTUBE>1, DIAM represents the diameter of a single tube.

NTUBE Number of tubes in the reactor (Default=1)

NPHASE Number of phases in MIXED substream:

NPHASE=1	One-phase calculation (Default)
NPHASE=2	Two-phase flash
NPHASE=3	Three-phase flash

PHASE Specifies the phase when NPHASE=1:

PHASE=V	Vapor (Default)
PHASE=L	Liquid

PRES Reactor pressure at inlet:

PRES > 0	Pressure
PRES ≤ 0	Pressure drop at inlet (Default=0)

PDROP Pressure drop through the reactor (Default=0)

U Heat transfer coefficient (per unit reactor wall area) between the coolant stream and the process stream, used for TCOOL-SPEC, CO-COOL, and COUNTER-COOL reactors.

MIX Substream mixing code for S prefix type reactors. Allowed only when TYPE=S-ADIABATIC, S-TCOOL-SPEC, S-CO-COOL, or S-COUNTER-COOL.

MIX=YES	Inlet MIXED and solid substreams are thermally mixed so they start out at the same temperature. (Default)
MIX=NO	Inlet substreams are not thermally mixed. If inlet substreams have different temperatures, calculations will begin with those temperatures.

FLASH

FLASH=YES	Process stream is flashed at all points along the reactor.
FLASH=NO	Flash performed only if necessary. Can be used by user-supplied subroutines. (Default)

UCM Heat transfer coefficient (per unit reactor wall area) between the coolant stream and the fluid phases. Use for S-TCOOL-SPEC, S-CO-COOL, and S-COUNTER-COOL reactors.

UCS Heat transfer coefficient (per unit reactor wall area) between the coolant stream and the solid phases. Use for S-TCOOL-SPEC, S-CO-COOL, and S-COUNTER-COOL reactors.

USM ..... Heat transfer coefficient (per unit reactor wall area) between the fluid phases and the solids phases. Use for S-ADIABATIC, S-TCOOL-SPEC, S-CO-COOL, and S-COUNTER-COOL reactors.

NPOINT..... Number of points along the length of the reactor in the reactor profiles printed in the block report. (Default=10)

MAX-NSTEP..... Number of integration steps allowed before block execution is terminated. (Default=1000)

HINIT ..... Initial step size of the integration variable; defined as a fraction of reactor length. In a few cases, with very fast reactions, you can use a number smaller than the default. (Default=0.01)

INT-TOL..... Convergence tolerance for integration procedure. (Default=$1x10^{-4}$)

CORR-METHOD..... Corrector convergence method:

CORR-METHOD=DIRECT	Direct substitution method. No derivatives are required.
CORR-METHOD=NEWTON	Newton method. Numerical derivatives are computed whenever a new Jacobian is required. (Default)

CORR-TOL-RATIO..... Ratio of the corrector tolerance to the integration tolerance (Default=0.1)

COMP-ATTR..... Flag used to determine whether to integrate component attributes, using the user-supplied subroutine:

COMP-ATTR=YES	Integrates component attributes
COMP-ATTR=NO	Does not integrate component attributes (Default)

SUBS-ATTR ..... Flag used to determine whether to integrate substream attributes, using the user-supplied subroutine:

SUBS-ATTR=YES	Integrates substream attributes
SUBS-ATTR=NO	Does not integrate substream attributes (Default)

ERR-METHOD ..... Error scaling method:

ERR-METHOD=STATIC	Constant scaling of tolerance (Default)
ERR-METHOD=DYNAMIC	Dynamic scaling of tolerance
ERR-METHOD=HYBRID	Enthalpy variables use dynamic scaling (scaled against their own values) while other variables use static scaling.

PDROP-OPTION ..... Pressure drop option:

PDROP-OPTION=PRES	User-supplied subroutine calculates pressure (Default)
PDROP-OPTION=PDROP	User-supplied subroutine calculates pressure drop (Default when COMP-ATTR or SUBS-ATTR=YES)

EB-TOL-RATIO ..... Ratio of energy balance (enthalpy) tolerance to integration tolerance. This parameter is only used when ERR-METHOD=HYBRID is selected. Increase this value to loosen energy balance tolerance. (Default=1)

INTEG-PARAMS Use to enter optional integration convergence parameters.

MAXSTEP ..... Maximum step size allowed in integration, as a fraction of reactor length

CUTOFF..... Cutoff value for dependent variables below which integration error is ignored. If you specify ERR-METHOD=STATIC, the cutoff value will not have an appreciable effect on the integrator performance. (Default=$1x10^{-10}$)

NONNEG ..... Non-negativity flag: YES or NO. Use to force integration variables to have positive values. (Default=NO)

COOLANT Use to enter coolant parameters for TCOOL-SPEC, CO-COOL, or COUNTER-COOL reactors. For TCOOL-SPEC reactors, only TEMP is entered.

PRES ..... **PRES > 0** Coolant pressure at inlet

PRES ≤ 0 Pressure drop at inlet (Default=0)

PDROP ..... Coolant pressure drop through the reactor (Default=0)

NPHASE ..... Number of phases for coolant flash calculations:

NPHASE=1 One-phase calculation

NPHASE=2 Two-phase flash (Default)

NPHASE=3 Three-phase flash

PHASE ..... Specifies the phase when NPHASE=1:

PHASE=V Vapor (Default)

PHASE=L Liquid

TEMP ..... For TCOOL-SPEC reactors, TEMP is the required constant coolant temperature. For COUNTER-COOL reactors, TEMP is the coolant outlet temperature.

VFRAC ..... Molar vapor fraction of the outlet coolant stream. Use for COUNTER-COOL reactors.

MAXIT ..... Maximum number of flash iterations for both process stream and coolant flash calculations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

TOL ..... Flash convergence tolerance for both process stream and coolant flash calculations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

T-SPEC Use to enter the temperature profile for T-SPEC reactors. RPLUG interpolates values for temperatures between specified locations. If you provide a temperature profile for only a portion of the reactor, RPLUG uses the final temperature for the remaining length. If you specify TYPE=T-SPEC and you do not enter the T-SPEC sentence, RPLUG uses the reactor inlet temperature as the temperature specification for the entire reactor length.

loc ..... Relative location in the reactor (for example, 0.5 for midpoint)

temp ..... Reactor temperature

REACTIONS Use to enter the IDs of the REACTIONS paragraphs that define the reactions. (See Chapter 6.) RPLUG can handle only kinetic type reactions.

reacid-list ..... List of reaction paragraph IDs

STOIC Use to specify the stoichiometric coefficients for each reaction. The use of this sentence is obsolete, but is maintained here for upward compatibility. Use the REACTIONS sentence instead.

reacno ..... Reaction number

ssid ..... Substream ID

cid ..... Component ID

coef ..... Stoichiometric coefficient (positive for products; negative for reactants)

RATE-CON Use to specify the pre-exponential factor, the temperature exponent, and the activation energy for each reaction. The use of this sentence is obsolete, but is maintained here for upward compatibility. Use the REACTIONS sentence instead.

reacno ..... Reaction number

pre-exp ..... Pre-exponential factor. Units must be in SI. (See the *Aspen Plus User Guide*.)

act-energy ..... Activation energy. (Units keyword is MOLE-ENTHALPY.)

temp-exponent ..... Temperature exponent for temperature in Kelvin (Default=0)

POWLAW-EXP Specifies the exponents for the components participating in each reaction. If the order of the reaction with respect to a component is zero, you do not have to enter that component. The use of this sentence is obsolete, but is maintained here for upward compatibility. Use the REACTIONS sentence instead.

reacno ..... Reaction number

cid..... Component ID

exponent ..... Exponent. Need not be an integer.

L2-COMPS Use to enter a list of components that are used to identify the second-liquid phase when NPHASE=3 and FREE-WATER=NO.

COMP-LIST..... List of component IDs in the second-liquid phase

L2-CUTOFF..... Mole fraction of second phase key component above which a phase is identified as the second-liquid phase, when only one liquid phase is present (Default=0.5)

REGR-POINTS Use to enter data sets and values for reactor locations for which the measurements have been specified using a PROFILE-DATA paragraph. (See Chapter 38.)

setno ..... Data set number

profdataid..... PROFILE-DATA paragraph ID

VALUE-LIST ..... List of locations in the reactor. Values must be in meters.

REGR-PARAM Use to enter the maximum number of measurement data points. (See Chapter 38.)

MAXPOINT..... Maximum number of measurement data points in all data sets referenced in the REGR-POINTS sentence

PROPERTIES Use to override the global or flowsheet section property specifications. If you supply one set of property specifications, it will be used for both process stream and coolant stream calculations. If you supply two sets, the first will be used for the process stream and the second for the coolant stream. Any option set name entered here must also be named in the PROPERTIES paragraph. (See Chapter 8.)

REPORT Use to override the default report options. You can use the standard REPORT options for use within a block (see Chapter 11) for RPLUG.

reportopt-list ..... The standard block report options (see Chapter 11), in addition to the following:

NOPROFILE	Suppresses profiles for temperature, pressure, and vapor fraction
NOCOMPS	Suppresses mole fraction profiles
USERVECS	Specifies printing of user integer and real arrays

PROP-REPORT Use to specify additional properties to be reported (in addition to temperature, pressure, vapor fraction, and mole fractions printed in the standard report).

propsetid-list ..... List of property set IDs. (See Chapter 41.)

PRINT-PLOT.....	**PRINT-PLOT=YES**	Produces print-plots of all tabulated properties
	PRINT-PLOT=NO	Does not produce print-plots (Default)
Y-SCALE.....	**Y-SCALE=STANDARD**	Uses linear scale on vertical axis of plots (Default)

		Y-SCALE=INVERSE	Uses inverse scale on vertical axis of plots
		Y-SCALE=LOG	Uses logarithmic scale on vertical axis of plots
	PLOT-HEADING		Heading up to 64 characters enclosed in quotes, printed at the top of the print-plot
	WIDE, GRID, INTERPOLATE		Plot options. Use to override defaults established by the PLOT-OPTIONS paragraph. (See Chapter 46.)
PLOT	Use to create plots of reactor temperature, pressure, vapor fraction, and/or mole fraction versus reactor length. Mole fractions of individual components or component groups can be reported.		
	plotno		Plot number
	plot-list		List of non-component-dependent properties to be plotted:
		TEMP	Reactor temperature
		PRES	Reactor pressure
		VFRAC	Reactor vapor fraction
	comp-plot		Keyword for component-dependent property to be plotted. Up to five components or groups will be printed on a plot.
		X, Y, Z	Liquid, vapor, and total mole fraction respectively
	groupid-list		List of component IDs and/or component group IDs
	Y-SCALE	**Y-SCALE=STANDARD**	Uses linear scale on vertical axis of plots (Default)
		Y-SCALE=INVERSE	Uses inverse scale on vertical axis of plots
		Y-SCALE=LOG	Uses logarithmic scale on vertical axis of plots
	PLOT-HEADING		Heading up to 64 characters enclosed in quotes, printed at the top of the print-plot
	WIDE, GRID, INTERPOLATE		Plot options. Use to override defaults established by the PLOT-OPTIONS paragraph. (See Chapter 46.)
PLOT-COOLANT	Use to create plots of coolant temperature (or composition) versus reactor length. Mole fractions of individual components or component groups can be reported.		
	plotno		Plot number
	plot-list		List of non-component-dependent property to be plotted:
		TEMP	Generates temperature plot
	comp-plot		Keyword for component-dependent property to be plotted:
		X, Y	Liquid and vapor mole fraction, respectively
	groupid-list		List of component IDs and/or component group IDs
	Y-SCALE	**Y-SCALE=STANDARD**	Uses linear scale on vertical axis of plots (Default)
		Y-SCALE=INVERSE	Uses inverse scale on vertical axis of plots
		Y-SCALE=LOG	Uses logarithmic scale on vertical axis of plots
	PLOT-HEADING		Heading up to 64 characters enclosed in quotes, printed at the top of the print-plot
	WIDE, GRID, INTERPOLATE		Plot options. Use to override defaults established by the PLOT-OPTIONS paragraph. (See Chapter 46.)
SUBROUTINE	Use to specify user-supplied pressure drop and heat transfer subroutines. For details on writing these user-supplied subroutines, see *Aspen Plus User Models*, Chapters 12 and 13.		
	KINETICS		The use of this keyword is obsolete, but is maintained here for upward compatibility. Use the REACTIONS paragraph instead. (See Chapter 6.)

PRES-DROP ..... User-supplied FORTRAN subroutine name for pressure drop calculations

QTRANS ..... User-supplied FORTRAN subroutine name for heat transfer calculations

USER-VECS

Use to define the length of arrays for user-supplied kinetic, pressure-drop, and heat transfer subroutines.

NINT ..... Length of integer parameter array for the user-supplied kinetic subroutine

NREAL ..... Length of real parameter array for the user-supplied kinetic subroutine

NIWORK ..... Length of integer workspace array for the user-supplied kinetic subroutine

NWORK ..... Length of real workspace array for the user-supplied kinetic subroutine

NINTP ..... Length of integer parameter array for the user-supplied pressure-drop subroutine

NREALP ..... Length of real parameter array for the user-supplied pressure-drop subroutine

NIWORKP ..... Length of integer workspace array for the user-supplied pressure-drop subroutine

NWORKP ..... Length of real workspace array for the user-supplied pressure-drop subroutine

NINTQ ..... Length of integer parameter array for the user-supplied heat transfer subroutine

NREALQ ..... Length of real parameter array for the user-supplied heat transfer subroutine

NIWORKQ ..... Length of integer workspace array for the user-supplied heat transfer subroutine

NWORKQ ..... Length of real workspace array for the user-supplied heat transfer subroutine

NUSER-PROF ..... Number of user-profile variables

INT, INTP, INTQ

Use to enter values for the integer parameter arrays of the user-supplied kinetic, pressure drop, and heat transfer subroutines.

value-list ..... List of integer values

REAL, REALP, REALQ

Use to enter values for the real parameter arrays of the user-supplied kinetic, pressure drop, and heat transfer subroutines.

value-list ..... List of real values

USERPROF

Use to enter labels and unit labels for user profile variables. These labels are used for reporting purposes only.

varno ..... User-profile variable number

LABEL ..... User-profile variable number label. The entered labels must be enclosed in quotes.

UNIT-LABEL ..... User-profile variable number unit label. The entered unit labels must be enclosed in quotes.

Accessing Variables in RPLUG

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	ID2	ID3	Element
PARAM	LENGTH, DIAM, NTUBE, PRES, PDROP, U, UCM, UCS, USM, HINIT, INT-TOL, CORR-TOL-RATIO	—	—	—	—
T-SPEC	TEMP†, LOC†	locno††	—	—	—
COOLANT	PRES, PDROP, TEMP, VFRAC, MAXIT, TOL	—	—	—	—
STOIC	COEF	reacno	ssid	cid	—
RATE-CON	PRE-EXP, ACT-ENERGY, TEMP-EXPONENT	reacno	—	—	—
POWLAW-EXP	EXPONENT	reacno	cid	—	—
INT	VALUE-LIST	—	—	—	†††
INTP	VALUE-LIST	—	—	—	†††
INTQ	VALUE-LIST	—	—	—	†††
REAL	VALUE-LIST	—	—	—	†††
REALP	VALUE-LIST	—	—	—	†††
REALQ	VALUE-LIST	—	—	—	†††

† You can also access variables using the VECTOR-DEF sentence. See Chapter 29.

†† locno is the entry number in the profile for the reactor location that is being accessed.

††† Position of a value in the value-list.

Block Results

Description	Sentence	Variable	ID1
Heat duty	PARAM	QCALC	—
Minimum temperature	PARAM	TMIN	—
Maximum temperature	PARAM	TMAX	—
Residence time	PARAM	RES-TIME	—
Reactor pressure	GENPROF	REAC-PRES†	locno
Reactor temperature	GENPROF	REAC-TEMP†	locno
Reactor location	GENPROF	REAC-LENGTH†	locno
Reactor residence time	GENPROF	REAC-RESTIME†	locno
Coolant pressure	GENPROF	COOLANT-PRES†	locno
Coolant inlet temperature	COOLANT	COOLANT-TIN	—
Coolant inlet vapor fraction	COOLANT	COOLANT-VIN	—

† You can also access variables using the VECTOR-DEF sentence. See Chapter 29.

RBATCH: Batch Reactor

Input Language for RBATCH

BLOCK **blockid** **RBATCH**
PARAM *keyword=value*

Keywords:

TYPE PRES TEMP DUTY VOLUME PRINT-TIME CYCLE-TIME FEED-TIME MAX-TIME MAX-NPOINT

Optional keywords:

DOWN-TIME NPHASE PHASE INT-TOL HINIT CORR-METHOD ERR-METHOD FLASH FLASH-MAXIT FLASH-TOL NPHASE-ACCUM PHASE-ACCUM REACSYS ADD-POINTS COMP-ATTR EB-TOL-RATIO

INTEG-PARAMS *keyword=value*

Keywords:

MAXSTEP IE-TOLFAC CUTOFF NONNEG

PCONV-OPT *keyword=value*

Keywords:

SOLVER MAXIT VOLUME-TOL PSTEP-INIT PRES-BAND PRES-LOWER PRES-UPPER FLASH-TOLFAC

T-PROF time temp / . . .
P-PROF time pres / . . .
DUTY-PROF time duty / . . .
FEED-PROF *keyword=value*

Keywords:

SID TIME FLOW

COOLANT *keyword=value*

Keywords:

TEMP U AREA

CONTROLLER *keyword=value*

Optional keywords:

GAIN INT-TIME DER-TIME

P-CONTROLLER *keyword=value*

Keywords:

P-SETPOINT P-GAIN

Optional keywords:

P-INT-TIME P-DER-TIME P-MAX-OUT

STOP stopno loc variable value from SSID=ssid COMP=cid &
PROPERTIES=prop-set

Locations:

REACTOR ACCUMULATOR VENT

Variables:

TIME MASS-FRAC MOLE-FRAC CONVERSION MOLES MASS VOLUME TEMP MOLE-FLOW MASS-FLOW VFRAC PRES PROP

VENT-OPTIONS P-OPEN=value
REACTIONS reacid-list
STOIC reacno ssid cid coef / cid coef / . . .
RATE-CON reacno pre-exp act-energy [temp-exponent]
POWLAW-EXP reacno cid exponent / cid exponent / . . .
L2-COMPS *keyword=value*

Keywords:

COMP-LIST L2-CUTOFF

REGR-POINT setno profdataid VALUE-LIST=value-list
REGR-PARAM MAXPOINT=value
REPORT reportopt-list

Special reportopts:

NOPROFILE USERVECS

PROP-REACTOR PROPERTIES=propsetid-list *keyword=value*
PROP-ACCUM PROPERTIES=propsetid-list *keyword=value*
PROP-VENT PROPERTIES=propsetid-list *keyword=value*

Optional keywords:

PRINT-PLOT Y-SCALE PLOT-HEADING WIDE GRID INTERPOLATE

PLOT-REACTOR plotno plot-list comp-plot=groupid-list *keyword=value*

Plots:

TEMP VFRAC MASS SETPOINT

Optional comp-plots:

X Y Z

Optional keywords:

Y-SCALE PLOT-HEADING WIDE GRID INTERPOLATE

PLOT-ACCUM plotno plot-list comp-plot=groupid-list *keyword=value*

Plots:

TEMP VFRAC MASS

Optional comp-plots:

X Y Z

Optional keywords:

Y-SCALE PLOT-HEADING WIDE GRID INTERPOLATE

PLOT-VENT plotno plot-list comp-plot=groupid-list *keyword=value*

Plot:

FLOW

Optional comp-plot:

Z

Optional keywords:

Y-SCALE PLOT-HEADING WIDE GRID INTERPOLATE

SUBROUTINE *keyword=value*

Keywords:

KINETICS HEAT-TRANS

USER-VECS *keyword=value*

Optional keywords:

NINT NREAL NIWORK NWORK NINTQ NREALQ NIWORKQ NWORKQ
NUSER-PROF

INT value-list **REAL value-list** **INTQ value-list** **REALQ value-list** **USER-PROF** *keyword=value*

Keywords:

ELEMENT LABEL UNIT-LABEL

Input Language Description for RBATCH

PARAM

Use to enter reactor type, output time interval, cycle time, maximum time, and optional algorithm parameters. You must enter either FEED-TIME or CYCLE-TIME. If the reactor batch charge stream is in a recycle loop, you must enter CYCLE-TIME. You can specify that one-, two-, or three-phase flash calculations be performed in the reactor. For two-phase calculations, the reaction can occur either in the liquid or in the vapor phase. When a continuous vapor vent is used, two-phase calculations are assumed, and the reactions are assumed to occur in the liquid phase.

TYPE	**TYPE=T-SPEC**	Constant temperature reactor
	TYPE=T-PROFILE	Reactor with time-temperature profile specified
	TYPE=DUTY-SPEC	Specified duty reactor
	TYPE=TCOOL-SPEC	Reactor with specified coolant temperature
	TYPE= DUTY-PROF	Reactor with time-duty profile specified
	TYPE=USER-DUTY	Reactor with user-supplied heat-transfer subroutine
PRES	**PRES > 0**	Reactor pressure
	PRES ≤ 0	Pressure drop from batch charge stream (Default=0)
TEMP	Set-point temperature of reactor, use for T-SPEC reactors	
DUTY	Reactor heat duty, use for DUTY-SPEC reactor (Default=0)	
VOLUME	Volume of the reactor	
PRINT-TIME	Time interval between profile points printed in the block report	

CYCLE-TIME ..... Reactor cycle time. If you enter CYCLE-TIME, this time is used for all feed and product stream conversions, regardless of the actual reaction time.
(Default=reaction time + DOWN-TIME)

FEED-TIME ..... Cycle time used to compute the actual batch charge

MAX-TIME ..... Upper limit on the reaction time

MAX-NPOINT ..... Number of output points generated if the upper limit on the reaction time is reached

DOWN-TIME..... Reactor down time used when you do not enter CYCLE-TIME. Total reactor cycle time is the reaction time required to reach a stopping criterion plus the down time. (Default=0)

NPHASE ..... NPHASE is used only when no vent product stream is present.

NPHASE=1	One-phase calculation (Default)
NPHASE=2	Two-phase flash
NPHASE=3	Three-phase flash

PHASE..... Specifies the phase when no vent product stream is present and NPHASE=1:

PHASE=V	Vapor
PHASE=L	Liquid (Default)

INT-TOL..... Convergence tolerance for integration routine (Default=$1x10^{-4}$)

HINIT ..... Initial step size (in seconds) used by the integration routine (Default=0.1)

CORR-METHOD..... Corrector convergence method:

CORR-METHOD=DIRECT	Direct substitution method
CORR-METHOD=NEWTON	Newton method (Default)

ERR-METHOD ..... Error scaling method:

ERR-METHOD=STATIC	Constant scaling of tolerance (Default)
ERR-METHOD=DYNAMIC	Dynamic scaling of tolerance
ERR-METHOD=HYBRID	Enthalpy variables use dynamic scaling (scaled against their own values) while other variables use static scaling.

FLASH ..... Switch to force flash calculations: YES or NO (Default=YES)

FLASH-MAXIT ..... Maximum number of iterations for flash calculations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

FLASH-TOL..... Convergence tolerance for flash calculations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

NPHASE-ACCUM..... Number of phases assumed in flash calculations in the vent accumulator. You must also specify the vent stream.

NPHASE-ACCUM=1	One-phase calculation (Default)
NPHASE-ACCUM=2	Two-phase flash calculation

PHASE-ACCUM ..... Specifies the phase of the vent stream when vent product stream is present and NPHASE-ACCUM=1:

PHASE-ACCUM=V	Vapor (Default)
PHASE-ACCUM=L	Liquid

REACSYS..... Switch to define whether any reactions are present: YES or NO (Default=YES)

ADD-POINTS ..... **ADD-POINTS=YES** Includes the times at which input profile points have been entered (Default)

ADD-POINTS=NO Does not include the times at which input profile points have been entered

COMP-ATTR ..... Flag used to determine whether to integrate component attributes, using the user-supplied kinetics subroutine

COMP-ATTR=YES Integrates component attributes

COMP-ATTR=NO Does not integrate component attributes (Default)

EB-TOL-RATIO ..... Ratio of energy balance (enthalpy) tolerance to integration tolerance. This parameter is only used when ERR-METHOD=HYBRID is selected. Increase this value to loosen energy balance tolerance. (Default=1)

INTEG-PARAMS Use to enter optional integration convergence parameters.

MAXSTEP ..... Maximum step size allowed in integration

IE-TOLFAC ..... Ratio of the tolerance for the error function used in the internal energy loop to the integration tolerance. The relative error in the calculated versus specified volume (or pressure, depending on whether the reactor is venting or not) is checked against this tolerance.The error is directly related to the error in the internal energy at any integration point, where the reactor contents are flashed at an enthalpy of H = U – PV. (Default=0.001)

CUTOFF ..... Cutoff value for dependent variables below which integration error is ignored. If you specify ERR-METHOD-STATIC, the cutoff value will not have an appreciable effect on the integrator performance. (Default=$1x10^{-10}$)

NONNEG..... Non-negativity flag: YES or NO. Use to force integrator variables to have positive values. (Default=NO)

PCONV-OPT Use to enter optional pressure convergence parameters.

SOLVER..... Solution scheme used in numerical search:

SOLVER=NEWTON Numerical search using the Newton method

SOLVER=ROOT1N Numerical search using modified secant method

SOLVER=ARCONS Numerical search using standard secant method

MAXIT..... Maximum number of iterations allowed (Default=300)

VOLUME-TOL..... Relative tolerance for convergence on volume (Default=$1x10^{-6}$)

PSTEP-INIT..... Initial step size for pressure search (Default=101.3 N/SQM)

PRES-BAND..... Band around previous pressure solution within which to search (Default=$1x10^{6}$ N/SQM)

PRES-LOWER ..... Lower bound on search (Default=10 N/SQM)

PRES-UPPER ..... Upper bound on search (Default=$1x10^{8}$ N/SQM)

FLASH-TOLFAC..... Flash tolerance factor (Default=0.001)

T-PROF Use to enter the time-temperature profile for T-PROFILE reactors. Linear interpolation is used for temperatures between the specified times.

time ..... Elapsed reaction time

temp ..... Reactor set-point temperature

P-PROF Use to enter the time-pressure profile. Linear interpolation is used for pressures between the specified times. You cannot use P-PROF when you specify the volume of reactor, VOLUME.

time ..... Elapsed reaction time

pres ..... Reactor pressure

DUTY-PROF Use to enter the time-duty profile for DUTY-PROFILE reactors. Linear interpolation is used for pressures between the specified times. You cannot use DUTY-PROF when you specify the volume of reactor, VOLUME.

time ..... Elapsed reaction time

duty ..... Reactor duty (rate of heat addition or removal)

FEED-PROF Use to enter flow rate profiles for continuous feed streams. All feed streams except the first, which is uniquely used to load the reactor, can be time-varying.

SID ..... Stream ID for continuous feed streams with user-specified flow rate profile

TIME ..... List of elapsed reaction time, in IN-UNITS for time

FLOW ..... List of mass flow rate at the corresponding time, in IN-UNITS for mass flow

COOLANT Use to enter coolant parameters for TCOOL-SPEC reactors.

TEMP..... Specified coolant temperature

U..... Heat transfer coefficient (per unit area) between the reactor contents and the constant temperature coolant

AREA..... Total area for heat transfer between the reactor contents and the constant temperature coolant

CONTROLLER Use to enter PID controller tuning parameters for T-SPEC and T-PROFILE reactors.

GAIN..... Proportional gain (Default=2500)

INT-TIME ..... Integral time constant (reset time) in seconds (Default=no integral action)

DER-TIME ..... Derivative time constant in seconds (Default=0)

P-CONTROLLER Use to simulate a pressure controller attached to the first continuous feed stream to the reactor. Use only when such a stream exists, reactor volume is specified, and reactor pressure is not specified.

P-SETPOINT..... Reactor pressure setpoint

P-GAIN ..... Proportional gain

P-INT-TIME..... Integral time constant (reset time) in seconds (Default=no integral action)

P-DER-TIME ..... Derivative time constant in seconds (Default=0)

P-MAX-OUT ..... Maximum mass flow rate of continuous feed stream

STOP Use to specify stop criteria. One STOP sentence is entered for each stop criterion. If you specify more than one stop criterion, the simulation is halted when any one of the stop criteria is reached. You can specify the stopping criterion variable to reach its specified value FROM-ABOVE or FROM-BELOW.

stopno ..... Stop criterion number

loc..... Location for the variable:

REACTOR In reactor

		ACCUMULATOR	In vent accumulator
		VENT	In continuous vent
	variable	Stop criterion variable:	
		TIME	Reaction time
		MASS-FRAC	Mass fraction of a component specified by COMP
		MOLE-FRAC	Mole fraction of a component specified by COMP
		CONVERSION	Conversion of a component specified by COMP
		MOLES	Total moles inside the reactor or the vent accumulator
		MASS	Total mass inside the reactor or the vent accumulator
		VOLUME	Total volume inside the reactor
		TEMP	Reactor temperature
		MOLE-FLOW	Vent mole flow rate
		MASS-FLOW	Vent mass flow rate
		VFRAC	Vapor fraction in the reactor
		PRES	Reactor pressure. If you enter a component ID, PRES is the corresponding component partial pressure.
		PROP	Prop-set property (defined in Chapter 41)
	value.....	Value of variable at which to stop reaction	
	from.....	**FROM-ABOVE**	Terminates reaction when variable value is reached from above
		FROM-BELOW	Terminates reaction when variable value is reached from below
	ssid.....	Substream ID	
	cid.....	Component ID. Use when *variable* is MOLE-FRAC, MASS-FRAC, or CONVERSION.	
	prop-set.....	Prop-set ID. (See Chapter 41.) Required when stop criterion *variable* is PROP.	
VENT-OPTIONS	Use to specify valve opening pressure option.		
	P-OPEN	Valve opening pressure	
REACTIONS	Use to enter the IDs of the REACTIONS paragraphs that define the reactions. (See Chapter 6.) RPLUG can handle only kinetic type reactions.		
	reacid-list	List of reaction paragraph IDs	
STOIC	Use to specify the stoichiometric coefficients for each reaction. The use of this sentence is obsolete, but is maintained here for upward compatibility. Use the REACTIONS sentence instead.		
	reacno	Reaction number	
	ssid.....	Substream ID	
	cid.....	Component ID	
	coef.....	Stoichiometric coefficient (positive for products; negative for reactants)	
RATE-CON	Use to specify the pre-exponential factor, the temperature exponent, and the activation energy for each reaction. The use of this sentence is obsolete, but is maintained here for upward compatibility. Use the REACTIONS sentence instead.		
	reacno	Reaction number	

pre-exp ..... Pre-exponential factor. Units must be in SI. (See the *Aspen Plus User Guide*)

act-energy ..... Activation energy. (Units keyword is MOLE-ENTHALPY.)

temp-exponent ..... Temperature exponent for temperature in Kelvin (Default=0)

POWLAW-EXP Specifies the exponents for the components participating in each reaction. If the order of the reaction with respect to a component is zero, you do not have to enter that component. The use of this sentence is obsolete, but is maintained here for upward compatibility. Use the REACTIONS sentence instead.

reacno ..... Reaction number

cid..... Component ID

exponent ..... Exponent. Does not have to be an integer.

L2-COMPS Use to enter a list of components that are used to identify the second-liquid phase when NPHASE=3 and FREE-WATER=NO.

COMP-LIST..... List of component IDs in the second-liquid phase

L2-CUTOFF..... Mole fraction of second phase key component above which a phase is identified as the second-liquid phase when only one liquid phase is present

REGR-POINTS Use to enter data sets and reaction times for which measurements have been specified in a PROFILE-DATA paragraph. (See Chapter 38.)

setno ..... Data set number

profdataid..... PROFILE-DATA paragraph ID

VALUE-LIST ..... List of reaction times. Values must be in seconds.

REGR-PARAM Use to enter the maximum number of measurement data points. (See Chapter 38.)

MAXPOINT..... Maximum number of measurement data points in all data sets referenced in the REGR-POINTS sentence

REPORT Use to override the report options. You can use the standard REPORT options for use within a block (see Chapter 11) for RBATCH.

reportopt-list ..... The standard block report options (see Chapter 11), in addition to the following:

NOPROFILE	Suppresses profiles for temperature, pressure, and vapor fraction
USERVECS	Specifies printing of user integer and real arrays

PROP-REACTOR, PROP-ACCUM, PROP-VENT Use to specify additional properties for the reactor, the vent accumulator, or the vent to be reported (in addition to temperature, pressure, vapor fraction, total mass, mole fractions, and setpoint temperature printed in the standard report).

propsetid-list ..... List of property set IDs. (See Chapter 41.)

PRINT-PLOT.....	**PRINT-PLOT=YES**	Produces print-plots of all tabulated properties
	PRINT-PLOT=NO	Does not produce print-plots of all tabulated properties (Default)
Y-SCALE.....	**Y-SCALE=STANDARD**	Uses linear scale on vertical axis of plots (Default)
	Y-SCALE=INVERSE	Uses inverse scale on vertical axis of plots
	Y-SCALE=LOG	Uses logarithmic scale on vertical axis of plots

PLOT-HEADING..... Heading up to 64 characters enclosed in quotes, printed at the top of the print-plot

	WIDE, GRID, INTERPOLATE		Plot options. Use to override defaults established by the PLOT-OPTIONS paragraph. (See Chapter 46.)
PLOT-REACTOR, PLOT-ACCUM, PLOT-VENT	Use to create plots of temperature, vapor fraction, total mass, setpoint temperature and/or mole fraction vs. reaction time. You can report mole fractions of individual components or component groups.		
	plotno		Plot number
	plot-list		List of non-component-dependent properties to be plotted:
		TEMP	Temperature
		VFRAC	Vapor fraction
		MASS	Total mass
		SETPOINT	Setpoint temperature
		FLOW	Vent molar flow rate
	comp-plot		Keyword for component-dependent property to be plotted. Up to five components or groups will be printed on a plot.
		X, Y, Z	Liquid, vapor, and total mole fraction respectively
	groupid-list		List of component IDs and/or component group IDs
	Y-SCALE	**Y-SCALE=STANDARD**	Uses linear scale on vertical axis of plots (Default)
		Y-SCALE=INVERSE	Uses inverse scale on vertical axis of plots
		Y-SCALE=LOG	Uses logarithmic scale on vertical axis of plots
	PLOT-HEADING		Heading up to 64 characters enclosed in quotes, printed at the top of the print-plot
	WIDE, GRID, INTERPOLATE		Plot options. Use to override defaults established by the PLOT-OPTIONS paragraph. (See Chapter 46.)
SUBROUTINE	Use to specify user-supplied kinetic and heat transfer subroutines. For details on writing these user-supplied subroutines, see *Aspen Plus User Models*, Chapter 14.		
	KINETICS		The use of this keyword is obsolete, but is maintained here for upward compatibility. Use the REACTIONS paragraph instead. (See Chapter 6.)
	HEAT-TRANS		User-supplied FORTRAN subroutine name for heat transfer calculations
USER-VECS	Use to define the length of arrays for user-supplied kinetic and heat transfer subroutines.		
	NINT		Length of integer parameter array for the user-supplied kinetic subroutine
	NREAL		Length of real parameter array for the user-supplied kinetic subroutine
	NIWORK		Length of integer workspace array for the user-supplied kinetic subroutine
	NWORK		Length of real workspace array for the user-supplied kinetic subroutine
	NINTQ		Length of integer parameter array for the user-supplied heat transfer subroutine
	NREALQ		Length of real parameter array for the user-supplied heat transfer subroutine
	NIWORKQ		Length of integer workspace array for the user-supplied heat transfer subroutine

NWORKQ..... Length of real workspace array for the user-supplied heat transfer subroutine

NUSER-PROF..... Number of user-profile variables

INT, INTQ

Use to enter values for the integer parameter arrays of the user-supplied kinetic and heat transfer subroutines.

value-list ..... List of integer values

REAL, REALQ

Use to enter values for the real parameter arrays of the user-supplied kinetic and heat transfer subroutines.

value-list ..... List of real values

USERPROF

Use to enter labels and unit labels for user profile variables. These labels will be used for reporting purposes only.

ELEMENT..... User-profile variable number

LABEL ..... User-profile variable number label. The labels must be enclosed in quotes.

UNIT-LABEL..... User-profile variable number unit label. The unit labels must be enclosed in quotes.

Accessing Variables in RBATCH

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	ID2	ID3	Element
PARAM	CYCLE-TIME, FEED-TIME, MAX-TIME, PRES, TEMP, DUTY, DOWN-TIME, INT-TOL, HINIT, FLASH-MAXIT, FLASH-TOL	—	—	—	—
COOLANT	TEMP, U, AREA	—	—	—	—
CONTROLLER	GAIN, INT-TIME, DER-TIME	—	—	—	—
P-CONTROLLER	P-SETPOINT, P-GAIN, P-INT-TIME, P-DER-TIME, P-MAX-OUT	—	—	—	—
STOP	VALUE	critno	—	—	—
STOIC	COEF	reacno	ssid	cid	—
RATE-CON	PRE-EXP, ACT-ENERGY, TEMP-EXPONENT	reacno	—	—	—
POWLAW-EXP	EXPONENT	reacno	cid	—	—
INT	VALUE-LIST	—	—	—	†
REAL	VALUE-LIST	—	—	—	†

† Position of a value in the INT or REAL value-list.

Block Results

Description	Sentence	Variable	ID1
Reaction time	PARAM	TIME	—
Time-averaged heat duty	RESULTS	QCALC	—
Heat duty per cycle	RESULTS	QCYCLE	—
Minimum temperature	RESULTS	TMIN	—
Maximum temperature	RESULTS	TMAX	—
Reactor pressure	GENPROF	REAC-PRES†	pointno
Reactor temperature	GENPROF	REAC-TEMP†	pointno
Elapsed time	GENPROF	REAC-TIME†	pointno
Vent molar flowrate	GENPROF	VENT-FLOW†	pointno
Total mass in reactor	GENPROF	REAC-MASS†	pointno
Total mass in vent accumulator	GENPROF	VENT-ACC-MAS†	pointno
Reactor accumulated duty	GENPROF	ACCUM-DUTY†	pointno
Reactor volume	GENPROF	REAC-VOLUME†	pointno
Reactor duty	GENPROF	REAC-DUTY†	pointno

† You can also access variables using the VECTOR-DEF sentence. See Chapter 29.

20 Pumps and Compressors

This chapter describes the input language for pump and compressor models. (For pressure changes only, you can use other models, such as HEATER.) The pump and compressor models change pressure when energy-related information, such as power requirement, is needed or known. The models are:

Model	Description	Purpose	Use
PUMP	Pump or hydraulic turbine	Changes stream pressure when the power requirement is needed or known	Pumps and hydraulic turbines
COMPR	Compressor or turbine	Changes stream pressure when the power requirement is needed or known	Polytropic compressors, polytropic positive displacement compressors, isentropic compressors, and isentropic turbines
MCOMPR	Multistage compressor or turbine	Changes stream pressure across multiple stages with intercoolers. Allows for liquid knockout streams from intercoolers.	Multistage polytropic compressors, polytropic positive displacement compressors, isentropic compressors, and isentropic turbines

PUMP: Pump/Hydraulic Turbine

Input Language for PUMP

```
BLOCK    blockid    PUMP
PARAM    keyword=value
```

Keywords:

PRES DELP PRATIO POWER

Optional keywords:

EFF DEFF NPHASE SUCT-AREA MAXIT TOL PUMP-TYPE HEAD-STATIC

```
PERFOR-PARAM    keyword=value
```

Optional keywords:

NCURVES ACT-SH-SPEED REF-SH-SPEED IMPELLER-DIA USER-CURVES SP-SPEED SUCT-SPEED SPEED-UNITS AFFEXPH AFFEXPE AFFEXPP

Optional keywords for head curves:

HEAD-FACTOR HEAD-NPOINT H-FLOW-VAR H-FLOW-UNIT HEAD-UNITS

Optional keywords for head coefficient curves

HEADC-FACTOR HEADC-NPOINT HC-FLOW-VAR HC-FLOW-UNIT

Optional keywords for brake horsepower curves:

POWER-FACTOR POWER-NPOINT PW-FLOW-VAR PW-FLOW-UNIT POWER-UNITS

Optional keywords for discharge pressure curves:

PRES-FACTOR PRES-NPOINT P-FLOW-VAR P-FLOW-UNIT PRES-UNITS

Optional keywords for pressure change curves:

PRAT-FACTOR PRAT-NPOINT PR-FLOW-VAR PR-FLOW-UNIT

Optional keywrods for pressure ratio curves

DELP-FACTOR DELP-NPOINT DP-FLOW-VAR DP-FLOW-UNIT DELP-UNITS

Optional keywords for efficiency curves:

EFF-FACTOR EFF-NPOINT EF-FLOW-VAR EF-FLOW-UNIT

Optional keywords for NPSHR curves:

NPSHR-FACTOR NPSHR-NPOINT HR-FLOW-VAR HR-FLOW-UNIT NPSHR-UNITS

```
HEAD-TABLE   curve   point   head   flow /  . . .
HEAD-POLY    curve   keyword=value  /  . . .
```

Keywords:

COEF1 COEF2 COEF3 COEF4

HEADC-TABLE curve point headc flow / . . .
HEADC-POLY curve *keyword=value* **/ . . .**

Keywords:

COEF1 COEF2 COEF3 COEF4

POWER-TABLE curve point power flow / . . .
POWER-POLY curve *keyword=value* **/ . . .**

Keywords:

COEF1 COEF2 COEF3 COEF4

PRES-TABLE curve point pres flow / . . .
PRES-POLY curve *keyword=value* **/ . . .**

Keywords:

COEF1 COEF2 COEF3 COEF4

PRATIO-TABLE curve point pratio flow / . . .
PRATIO-POLY curve *keyword=value* **/ . . .**

Keywords:

COEF1 COEF2 COEF3 COEF4

DELP-TABLE curve point delp flow / . . .
DELP-POLY curve *keyword=value* **/ . . .**

Keywords:

COEF1 COEF2 COEF3 COEF4

EFF-TABLE curve point eff flow / . . .
EFF-POLY curve *keyword=value* **/ . . .**

Keywords:

COEF1 COEF2 COEF3 COEF4

NPSHR-TABLE curve point npshr flow / . . .
NPSHR-POLY curve *keyword=value* **/ . . .**

Keywords:

COEF1 COEF2 COEF3 COEF4

SHAFT-SPEED curve shaft-speed / . . .
SUBROUTINE CURVES=subrname
USER-VECS *keyword=value*

Optional keywords:

NINT NREAL NIWORK NWORK

INT value-list
REAL value-list
UTILITY UTILITY-ID=*utilityid*

Input Language Description for PUMP

PARAM

Use to specify pump efficiencies and optional flash convergence. You can also specify driver efficiency. You can use an inlet work stream to provide a power specification.

PRES	Outlet pressure	
DELP	Pressure increase for pumps or pressure decrease for turbines.	
PRATIO	Pressure ratio (outlet pressure/inlet pressure)	
POWER	Power supplied to a pump or power produced by a turbine. Work streams use the opposite convention.	
PUMP-TYPE	**PUMP-TYPE=PUMP**	Model type is pump (Default).
	PUMP-TYPE=TURBINE	Model type is turbine.
EFF	Efficiency. For pump, EFF=Fluid horsepower/Brake horsepower For turbine, EFF=Brake horsepower/Fluid horsepower (Default=value calculated using efficiency curves for water in a centrifugal pump)	
DEFF	Driver efficiency. For pump, DEFF=Brake horsepower/Electrical horsepower For turbine, DEFF=Electrical horsepower/Brake horsepower (Default=1)	
NPHASE	**NPHASE=1**	Liquid-phase calculations only (Default)
	NPHASE=2	Two-phase flash
	NPHASE=3	Three-phase flash
SUCT-AREA	Cross-sectional area of the suction nozzle used in calculating net positive suction head (NPSH)	
MAXIT	Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	
TOL	Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	
HEAD-STATIC	Hydraulic static head	

PERFOR-PARAM

Use to enter optional parameters related to pump performance curves.

NCURVES	Number of pump performance curves. If: • A single curve is supplied, it can be used to rate a pump at a given speed • A reference shaft speed is known, affinity laws will be used to scale the performance • Multiple curves are supplied, linear interpolation is performed between curves to find the performance at operating point	
ACT-SH-SPEED	Pump shaft speed	
REF-SH-SPEED	Reference pump shaft speed. Use when affinity laws are applied to determine pump performance.	
IMPELLER-DIA	Diameter of the pump's impeller	
USER-CURVES	Specifies the type of performance variable supplied by a user subroutine	
	USER-CURVE=HEAD	Head
	USER-CURVE= HEAD-COEF	Head coefficient
	USER-CURVE=POWER	Power

	USER-CURVE=PRES	Discharge pressure
	USER-CURVE=PRATIO	Pressure ratio
	USER-CURVE=DELP	Pressure change

SP-SPEED..... Specific speed at the best efficiency point

$$\text{SP-SPEED} = \text{ACT-SH-SPEED} * \text{FLOWRATE}^{0.5} / \text{HEAD}^{0.75}$$

SUCT-SPEED ..... Suction specific speed at the best efficiency point

$$\text{SUCT-SPEED} = \text{ACT-SH-SPEED} * \text{FLOWRATE}^{0.5} / \text{NPSHR}^{0.75}$$

SPEED-UNITS..... Units used in determining specific speed and suction specific speed

SPEED-UNITS=US	Units for ACT-SH-SPEED, FLOWRATE and HEAD (or NPSHR) are RPM, GAL/MIN, and FT respectively (Default)
SPEED-UNITS=METRIC	Units for ACT-SH-SPEED, FLOWRATE and HEAD (or NPSHR) are RPM, CUM/HR, and M respectively

AFFEXPH ..... Affinity law exponent for head (Default=2.0)

AFFEXPE ..... Affinity law exponent for efficiency (Default=1.0)

AFFEXPP ..... Affinity law exponent for brake horsepower (Default=3.0)

HEAD-FACTOR..... Scaling factor applied to head values calculated from either tabular (HEAD-TABLE) or polynomial (HEAD-POLY) data (Default=1)

HEAD-NPOINT..... Maximum number of data points in a curve when head versus flow curves are specified in a table

H-FLOW-VAR..... Independent flow variable used in head versus flow curves:

H-FLOW-VAR=VOL-FLOW	Volume flow
H-FLOW-VAR= MASS-FLOW	Mass flow

H-FLOW-UNIT ..... Units of the independent flow variable in head versus flow curves

HEAD-UNITS ..... Units of head data in head versus flow curves

HEADC-FACTOR..... Scaling factor applied to head coefficient values calculated from either tabular (HEADC-TABLE) or polynomial (HEADC-POLY) data of performance curves (Default=1)

HEADC-NPOINT..... Maximum number of data points in a curve when head coefficient versus flow curves are specified in a table

HC-FLOW-VAR..... Independent flow variable used in head coefficient versus flow curves:

H-FLOW-VAR= "VOL-FLOW/N"	Volume flow per shaft speed in RPM, or specific flow
H-FLOW-VAR= FLOW-COEFF	Flow coefficient

HC-FLOW-UNIT ..... Units of the independent flow variable in head coefficient versus flow curves

POWER-FACTOR..... Scaling factor applied to power values calculated from either tabular (POWER-TABLE) or polynomial (POWER-POLY) data (Default=1)

POWER-NPOINT..... Maximum number of data points in a curve when power versus flow curves are specified in a table

PW-FLOW-VAR..... Independent flow variable used in power versus flow curves:

PW-FLOW-VAR= VOL-FLOW Volume flow

PW-FLOW-VAR= MASS-FLOW Mass flow

PW-FLOW-UNIT ..... Units of the independent flow variable in power versus flow curves

POWER-UNITS ..... Units of power data in power versus flow curves

PRES-FACTOR ..... Scaling factor applied to discharge pressure values calculated from either tabular (PRES-TABLE) or polynomial (PRES-POLY) data (Default=1)

PRES-NPOINT ..... Maximum number of data points in a curve when discharge pressure versus flow curves are specified in a table

P-FLOW-VAR..... Independent flow variable used in discharge pressure versus flow curves:

P-FLOW-VAR= VOL-FLOW Volume flow

P-FLOW-VAR= MASS-FLOW Mass flow

P-FLOW-UNIT ..... Units of the independent flow variable in discharge pressure versus flow curves

PRES-UNITS..... Units of pressure data in discharge pressure versus flow curves

PRAT-FACTOR ..... Scaling factor applied to pressure ratio values calculated from either tabular (PRATIO-TABLE) or polynomial (PRATIO-POLY) data (Default=1)

PRAT-NPOINT ..... Maximum number of data points in a curve when pressure ratio versus flow curves are specified in a table

PR-FLOW-VAR..... Independent flow variable used in pressure ratio versus flow curves:

PR-FLOW-VAR= VOL-FLOW Volume flow

PR-FLOW-VAR= MASS-FLOW Mass flow

PR-FLOW-UNIT ..... Units of the independent flow variable in pressure ratio versus flow curves

DELP-FACTOR ..... Scaling factor applied to pressure change values calculated from either tabular (DELP-TABLE) or polynomial (DELP-POLY) data (Default=1)

DELP-NPOINT ..... Maximum number of data points in a curve when pressure change versus flow curves are specified in a table

DP-FLOW-VAR..... Independent flow variable used in pressure change versus flow curves:

DP-FLOW-VAR= VOL-FLOW Volume flow

DP-FLOW-VAR= MASS-FLOW Mass flow

DP-FLOW-UNIT ..... Units of the independent flow variable in pressure change versus flow curves

DELP-UNITS..... Units of pressure change data in pressure change versus flow curves

EFF-FACTOR..... Scaling factor applied to efficiency values calculated from either tabular (EFF-TABLE) or polynomial (EFF-POLY) data (Default=1)

EFF-NPOINT..... Maximum number of data points in a curve when efficiency versus flow curves are specified in a table

EF-FLOW-VAR ..... Independent flow variable used in efficiency versus flow curves:

EF-FLOW-VAR= VOL-FLOW	Volume flow
EF-FLOW-VAR= MASS-FLOW	Mass flow
EF-FLOW-VAR= "VOL-FLOW/N"	Volume flow per shaft speed in RPM or specific speed
EF-FLOW-VAR= FLOW-COEFF	Flow coefficient

EF-FLOW-UNIT..... Units of the independent flow variable in efficiency versus flow curves

NPSHR-FACTOR ..... Scaling factor applied to required NPSH values calculated from either tabular (NPSHR-TABLE) or polynomial (NPSHR-POLY) data (Default=1)

NPSHR-NPOINT ..... Maximum number of data points in a curve when required NPSH versus flow curves are specified in a table

HR-FLOW-VAR ..... Independent flow variable used in required NPSH versus flow curves:

HR-FLOW-VAR= VOL-FLOW	Volume flow
HR-FLOW-VAR= MASS-FLOW	Mass flow
HR-FLOW-VAR= "VOL-FLOW/N"	Volume flow per shaft speed in RPM or specific speed
HR-FLOW-VAR= FLOW-COEFF	Flow coefficient

HR-FLOW-UNIT..... Units of the independent flow variable in required NPSH versus flow curves

NPSHR-UNITS..... Units of head data in required NPSH versus flow curves

HEAD-TABLE

Use to enter values of head developed versus suction flow rate in a table. You must also specify HEAD-NPOINT, HEAD-UNITS, H-FLOW-VAR, and H-FLOW-UNIT in the PERFOR-PARAM sentence. (See Notes 6 and 7.)

curve ..... Curve number

point..... Row number within a table

head ..... Head developed.

flow ..... Suction flow rate (volumetric or mass)

HEAD-POLY

Use to enter polynomial coefficients to calculate head developed as a function of suction flow rate. You must also specify H-FLOW-VAR and H-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 6.) The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Suction flow rate (volumetric or mass)

Y = Head developed

curve ..... Curve number

COEF1 ..... First coefficient of head versus flow polynomial

COEF2 ..... Second coefficient of head versus flow polynomial

COEF3 ..... Third coefficient of head versus flow polynomial

COEF4 ..... Fourth coefficient of head versus flow polynomial

HEADC-TABLE

Use to enter values of head coefficient versus either suction flow rate per shaft speed in rpm or flow coefficient, in a table. You must also specify HEADC-NPOINT, HC-FLOW-VAR, and HC-FLOW-UNIT (if applicable) in the PERFOR-PARAM sentence. (See Notes 6, 7, and 8.)

curve ..... Curve number

point ..... Row number within a table

head-coeff ..... Head coefficient.

flow ..... Suction flow rate per shaft speed in rpm, or value of flow coefficient

HEADC-POLY

Use to enter polynomial coefficients to calculate head coefficient as a function of either suction flow rate per shaft speed in rpm or flow coefficient, in polynomial form. You must also specify HC-FLOW-VAR and HC-FLOW-UNIT (if applicable) in the PERFOR-PARAM sentence. (See Notes 6 and 8.) The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Volumetric flow rate per shaft speed in rpm or flow coefficient

Y = Head coefficient

curve ..... Curve number

COEF1 ..... First coefficient of head coefficient versus flow polynomial

COEF2 ..... Second coefficient of head coefficient versus flow polynomial

COEF3 ..... Third coefficient of head coefficient versus flow polynomial

COEF4 ..... Fourth coefficient of head coefficient versus flow polynomial

POWER-TABLE

Use to enter values of power supplied versus suction flow rate in a table. You must also specify POWER-NPOINT, POWER-UNITS, PW-FLOW-VAR, and PW-FLOW-UNIT in the PERFOR-PARAM sentence. (See Notes 6 and 7.)

curve ..... Curve number

point ..... Row number within a table

power ..... Power supplied

flow ..... Suction flow rate (volumetric or mass)

POWER-POLY

Use to enter polynomial coefficients to calculate the power supplied as a function of suction flow rate. You must also specify POWER-UNITS, PW-FLOW-VAR, and PW-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 6.) The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Suction flow rate (volumetric or mass)

Y = Power supplied

curve ..... Curve number

COEF1 ..... First coefficient of power versus flow polynomial

COEF2 ..... Second coefficient of power versus flow polynomial

COEF3 ..... Third coefficient of power versus flow polynomial

COEF4 ..... Fourth coefficient of power versus flow polynomial

PRES-TABLE

Use to enter values of discharge pressure versus suction flow rate in a table. You must also specify PRES-NPOINT, PRES-UNITS, P-FLOW-VAR, and P-FLOW-UNIT in the PERFOR-PARAM sentence. (See Notes 6 and 7.)

curve ..... Curve number

point ..... Row number within a table

pres ..... Discharge pressure

flow ..... Suction flow rate (volumetric or mass)

PRES-POLY

Use to enter polynomial coefficients to calculate discharge pressure as a function of suction flow rate. You must also specify PRES-UNITS, P-FLOW-VAR, and P-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 6.) The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Suction flow rate (volumetric or mass)

Y = Discharge pressure

curve ..... Curve number

COEF1 ..... First coefficient of pressure versus flow polynomial

COEF2 ..... Second coefficient of pressure versus flow polynomial

COEF3 ..... Third coefficient of pressure versus flow polynomial

COEF4 ..... Fourth coefficient of pressure versus flow polynomial

PRATIO-TABLE

Use to enter pressure ratio (discharge pressure/suction pressure) versus suction flow rate in a table. You must also specify PRAT-NPOINT, PR-FLOW-VAR, and PR-FLOW-UNIT in the PERFOR-PARAM sentence. (See Notes 6 and 7.)

curve ..... Curve number

point ..... Row number within a table

pratio ..... Pressure ratio

flow ..... Suction flow rate (volumetric or mass)

PRATIO-POLY

Use to enter polynomial coefficients to calculate pressure ratio (discharge pressure/suction pressure) as a function of suction flow rate. You must also specify PR-FLOW-VAR and PR-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 6.) The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Suction flow rate (volumetric or mass)

Y = Pressure ratio

curve ..... Curve number

COEF1 ..... First coefficient of pratio versus flow polynomial

COEF2 ..... Second coefficient of pratio versus flow polynomial

COEF3 ..... Third coefficient of pratio versus flow polynomial

COEF4 ..... Fourth coefficient of pratio versus flow polynomial

DELP-TABLE

Use to enter values of pressure change (discharge pressure/suction pressure) versus suction flow rate in a table. You must also specify DELP-NPOINT, DELP-UNITS, DP-FLOW-VAR, and DP-FLOW-UNIT in the PERFOR-PARAM sentence.(See Notes 6 and 7.)

curve ..... Curve number

point ..... Row number within a table

delp ..... Pressure change

flow ..... Suction flow rate (volumetric or mass)

DELP-POLY

Use to enter polynomial coefficients to calculate pressure change (discharge pressure-suction pressure) as a function of suction flow rate. You must also specify DELP-UNITS, DP-FLOW-VAR, and DP-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 6.) The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Suction flow rate (volumetric or mass)

Y = Pressure change

curve ..... Curve number

COEF1 ..... First coefficient of delp versus flow polynomial

COEF2 ..... Second coefficient of delp versus flow polynomial

COEF3 ..... Third coefficient of delp versus flow polynomial

COEF4 ..... Fourth coefficient of delp versus flow polynomial

EFF-TABLE

Use to enter values of efficiency versus suction flow rate in a table. You must also specify EFF-NPOINT, EF-FLOW-VAR, and EF-FLOW-UNIT in the PERFOR-PARAM sentence. (See Notes 6, 7 and 9.)

curve ..... Curve number

point ..... Row number within a table

eff ..... Efficiency

flow ..... Suction flow rate (volumetric, mass, specific flow, or flow coefficient)

EFF-POLY

Use to enter polynomial coefficients to calculate efficiency as a function of suction flow rate. You must also specify EF-FLOW-VAR and EF-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 6.) The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Suction flow rate (volumetric, mass, specific flow, or flow coefficient)

Y = Efficiency

curve ..... Curve number

COEF1 ..... First coefficient of efficiency versus flow polynomial

COEF2 ..... Second coefficient of efficiency versus flow polynomial

COEF3 ..... Third coefficient of efficiency versus flow polynomial

COEF4 ..... Fourth coefficient of efficiency versus flow polynomial

NPSHR-TABLE Use to enter values of efficiency versus suction flow rate in a table. You must also specify NPSHR-NPOINT, NPSHR-UNITS, HR-FLOW-VAR, and HR-FLOW-UNIT in the PERFOR-PARAM sentence. (See Notes 6 and 7.)

curve ..... Curve number

point ..... Row number within a table

npshr ..... NPSH required

flow ..... Suction flow rate (volumetric, mass, specific flow, or flow coefficient)

NPSHR-POLY Use to enter polynomial coefficients to calculate efficiency as a function of suction flow rate. You must also specify NPSHR-UNITS, HR-FLOW-VAR and HR-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 6.) The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Suction flow rate (volumetric, mass, specific flow, or flow coefficient)

Y = NPSH required

curve ..... Curve number

COEF1 ..... First coefficient of NPSH required versus flow polynomial

COEF2 ..... Second coefficient of NPSH required versus flow polynomial

COEF3 ..... Third coefficient of NPSH required versus flow polynomial

COEF4 ..... Fourth coefficient of NPSH required versus flow polynomial

SHAFT-SPEED Use to enter pump shaft speeds when multiple performance curves, at multiple shaft speeds, are available. (See Note 10.)

curve ..... Curve number

shaft-speed..... Shaft speed

SUBROUTINE Use to specify user-supplied subroutine for calculating performance curves. You must specify the type of curve using the USER-CURVES keyword in the PERFOR-PARAM sentence. The user subroutine must also calculate efficiency, whenever it is used to calculate any other performance variable. See *Aspen Plus User Models*, Chapter 22, for information about writing user-supplied subroutines for performance curves.

CURVES..... Name of user-supplied FORTRAN subroutine for performance curve calculations

USER-VECS Use to define the length of arrays for user-supplied performance curve subroutines.

NINT ..... Length of integer parameter array for the user-supplied performance curve subroutine

NREAL..... Length of real parameter array for the user-supplied performance curve subroutine

NIWORK ..... Length of integer workspace array for the user-supplied performance curve subroutine

NWORK ..... Length of real parameter array for the user-supplied performance curve subroutine

INT Use to enter values for the integer parameter array of the user-supplied performance curve subroutine.

value-list ..... List of integer values

REAL Use to enter values for the real parameter array of the user-supplied performance curve subroutine.

value-list ..... List of real values

UTILITY Use to specify an optional utility to provide heating or cooling duty.

UTILITY-ID ..... Utility ID.

Accessing Variables in PUMP

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for a PUMP block.

Block Input

Sentence	Variables	ID1	ID2
PARAM	PRES, DELP, PRATIO, POWER, EFF, DEFF, MAXIT, TOL, SUCT-AREA, HEAD-STATIC		
PERFOR-PARAM	IMPELLER-DIA, AFFEXPH, AFFEXPE, AFFEXPP, HEAD-FACTOR, HEADC-FACTOR, POWER-FACTOR, PRES-FACTOR, PRAT-FACTOR, DELP-FACTOR, EFF-FACTOR, HR-FACTOR, SP-SPEED, SUCT-SPEED, ACT-SH-SPEED, REF-SH-SPEED		
HEAD-TABLE	HEAD, FLOW	curve	point
HEAD-POLY	COEF1, COEF2, COEF3, COEF4	curve	—
HEADC-TABLE	HEAD-COEF, FLOW	curve	point
HEADC-POLY	COEF1, COEF2, COEF3, COEF4	curve	—
POWER-TABLE	POWER, FLOW	curve	point
POWER-POLY	COEF1, COEF2, COEF3, COEF4	curve	—
PRES-TABLE	PRES, FLOW	curve	point
PRES-POLY	COEF1, COEF2, COEF3, COEF4	curve	—
PRATIO-TABLE	PRATIO, FLOW	curve	point
PRATIO-POLY	COEF1, COEF2, COEF3, COEF4	curve	—
DELP-TABLE	DELP, FLOW	curve	point
DELP-POLY	COEF1, COEF2, COEF3, COEF4	curve	—
EFF-TABLE	EFFICIENCY, FLOW	curve	point
EFF-POLY	COEF1, COEF2, COEF3, COEF4	curve	—
NPSHR-TABLE	NPSHR, FLOW	curve	point
NPSHR-POLY	COEF1, COEF2, COEF3, COEF4	curve	—
SHAFT-SPEED	SHAFT-SPEED	curve	—

Block Results

Description	Sentence	Variable
Fluid horsepower	RESULTS	FLUID-POWER
Brake horsepower	RESULTS	BRAKE-POWER
Electrical horsepower	RESULTS	ELEC-POWER
NPSH available at the pump suction nozzle	RESULTS	NPSH-AVAIL
NPSH required	RESULTS	NPSH-REQ
Net work	RESULTS	NET-WORK
Calculated pressure change	RESULTS	DELP-CALC
Calculated volumetric flow rate	RESULTS	VOLUME-FLOW
Efficiency used	RESULTS	CALCULATED-E
Calculated specific speed	PERF-RESULTS	SP-SPEED-CAL
Calculated suction specific speed	PERF-RESULTS	SUCT-SPEED-C
Head coefficient	PERF-RESULTS	HEAD-COEFF
Flow-coefficient	PERF-RESULTS	FLOW-COEFF

COMPR: Compressor/Turbine

Input Language for COMPR

BLOCK **blockid** **COMPR**
PARAM *keyword=value*

Keywords:

TYPE **PRES** **DELP** **PRATIO** **POWER**

Optional keywords:

MODEL-TYPE **TEMP** **PEFF** **SEFF** **MEFF** **CLFR** **NPHASE** **SB-MAXIT** **SB-TOL** **MAXIT** **TOL** **PS-FLASH** **INT-METHOD** **INT-STEP** **PRAT-STEP** **PRAT-FINAL** **INTERVALS** **PLOSS-FACTOR** **PLOSS-OFFSET** **PL-FLOW-UNIT** **PLOSS-UNITS** **PL-SP-UNIT**

PERFOR-PARAM *keyword=value*

Optional keywords:

SUCT-NOZ-DIA **SUCT-K-FACT** **GPSA-BASIS** **NCURVES** **EXTRAPOLATE** **CALC-SPEED** **ACT-SH-SPEED** **IMPELLER-DIA** **USER-CURVES** **REF-SH-SPEED** **FANEXPH** **FANEXPE** **FANEXPP** **SPLINE-FIT** **OPT-DESIGN** **CORR-FLOW** **CURVE-DIM** **DEF-PRATIO** **GEAR-RATIO** **PIN-DESIGN** **TIN-DESIGN** **PIN-UNITS** **TIN-UNITS** **GAS-CONST-UNIT**

Optional keywords for head curves:

HEAD-FACTOR **HEAD-OFFSET** **HEAD-NPOINT** **H-FLOW-VAR** **H-FLOW-UNIT** **HEAD-UNITS** **HEAD-SP-UNIT** **ACTUAL-HEAD**

Optional keywords for head coefficient curves:

HEADC-FACTOR **HEADC-OFFSET** **HEADC-NPOINT** **HC-FLOW-VAR** **HC-FLOW-UNIT** **ACTUAL-HEADC**

Optional keywords for power curves:

POWER-FACTOR POWER-OFFSET POWER-NPOINT PW-FLOW-VAR PW-FLOW-UNIT POWER-UNITS

Optional keywords for discharge pressure curves:

PRES-FACTOR PRES-OFFSET PRES-NPOINT P-FLOW-VAR P-FLOW-UNIT PRES-UNITS

Optional keywords for pressure ratio curves:

PRAT-FACTOR PRAT-OFFSET PRAT-NPOINT PR-FLOW-VAR PR-FLOW-UNIT

Optional keywords for pressure change curves:

DELP-FACTOR DELP-OFFSET DELP-NPOINT DP-FLOW-VAR DP-FLOW-UNIT DELP-UNITS

Optional keywords for efficiency curves:

EFF-FACTOR EFF-OFFSET EFF-NPOINT EF-FLOW-VAR EF-FLOW-UNIT EFF-SP-UNIT

Optional keywords for surge volume curves:

SURGE-FACTOR SURGE-OFFSET SURGE-UNITS SG-SP-UNIT

HEAD-TABLE curve point head flow / ....
HEAD-POLY curve *keyword=value* **/ ...**

Keywords:

COEF1 COEF2 COEF3 COEF4 SURGE STONEWALL

HEADC-TABLE curve point head-coeff flow / ...
HEADC-POLY curve *keyword=value* **/ ...**

Keywords:

COEF1 COEF2 COEF3 COEF4 SURGE STONEWALL

POWER-TABLE curve point power flow / ....
POWER-POLY curve *keyword=value* **/ ...**

Keywords:

COEF1 COEF2 COEF3 COEF4 SURGE STONEWALL

PRES-TABLE curve point pres flow / ....
PRES-POLY curve *keyword=value* **/ ...**

Keywords:

COEF1 COEF2 COEF3 COEF4 SURGE STONEWALL

PRATIO-TABLE curve point pratio flow / ....
PRATIO-POLY curve *keyword=value* **/ ...**

Keywords:

COEF1 COEF2 COEF3 COEF4 SURGE STONEWALL

DELP-TABLE curve point delp flow / ....

```
DELP-POLY    curve    keyword=value  /  ...
```

Keywords:

COEF1 COEF2 COEF3 COEF4 SURGE STONEWALL

```
EFF-TABLE    curve    point    eff    flow  /  ....
EFF-POLY     curve    keyword=value  /  ...
```

Keywords:

COEF1 COEF2 COEF3 COEF4

```
SHAFT-SPEED    curve    shaft-speed  /  ...
MACH-NO    curve    mach-no  /  ...
HEAD-CORR    keyword=value
```

Keywords:

COEF1 COEF2 COEF3 COEF4 COEF5 COEF6 COEF7 COEF8

```
EFF-CORR    keyword=value
```

Keywords:

COEF1 COEF2 COEF3 COEF4 COEF5 COEF6 COEF7 COEF8

```
SURGE-POLY    keyword=value
```

Keywords:

COEF1 COEF2 COEF3

```
PLOSS-POLY    keyword=value
```

Keywords:

COEF1 COEF2 COEF3

```
SUBROUTINE    CURVES=subrname
USER-VECS    keyword=value
```

Optional keywords:

NINT NREAL NIWORK NWORK

```
INT    value-list
REAL    value-list
UTILITY    UTILITY-ID=utilityid
```

Input Language Description for COMPR

PARAM

Use to enter compressor specifications, efficiencies, and optional flash convergence parameters. You can use an inlet work stream to provide a power specification.

MODEL-TYPE	**MODEL-TYPE= COMPRESSOR**	Model type is compressor. (Default)
	MODEL-TYPE= TURBINE	Model type is turbine.
TYPE	**TYPE=ISENTROPIC**	Isentropic compressor/turbine (only this option is allowed for turbines)

	TYPE=POS-DISP	Polytropic positive-displacement compressor calculations
	TYPE=ASME-POLYTROPIC	Polytropic compressor calculations using the ASME method[3]
	TYPE=ASME-ISENTROPIC	Isentropic compressor calculations using the ASME method[3]
	TYPE=GPSA-POLYTROPIC	Polytropic compressor calculations using the GPSA method[4]
	TYPE=GPSA-ISENTROPIC	Isentropic compressor calculations using the GPSA method[4]
	TYPE=INT-POLYTROPIC	Polytropic compressor calculations using the piecewise integration method (see Note 12.)
	TYPE=INT-POS-DISP	Polytropic positive-displacement compressor calculation using the integration method (see Note 12.)

PRES ..... Outlet pressure

DELP ..... Pressure change. When MODEL-TYPE=COMPRESSOR, DELP > 0 is pressure increase and DELP ≤ 0 is pressure decrease. You can use DELP ≤ 0 only when TYPE=ISENTROPIC. When MODEL-TYPE=TURBINE, DELP is pressure decrease and must be greater than or equal to 0.

PRATIO ..... Pressure ratio (outlet pressure/inlet pressure)

POWER ..... Power input. When MODEL-TYPE=COMPRESSOR, power supplied to the compressor is positive. Power produced by a turbine is negative. Work streams use the opposite convention. When MODEL-TYPE=TURBINE, POWER is power produced and must be positive.

TEMP..... Outlet temperature. Use when TYPE=GPSA-POLYTROPIC, POS-DISP, or ASME-POLYTROPIC.

PEFF..... Polytropic efficiency as defined in Note 1. Use when TYPE=GPSA-POLYTROPIC, POS-DISP, or ASME-POLYTROPIC. (Default=0.72)

SEFF..... Isentropic efficiency as defined in Note 2. Use only when TYPE=ISENTROPIC, GPSA-ISENTROPIC, or ASME-ISENTROPIC. (Default=0.72)

MEFF..... Mechanical efficiency as defined in Note 3. (Default=1)

CLFR ..... Clearance fraction. Use only when TYPE=POS-DISP. (Default=0.5)

NPHASE .....

NPHASE=1	Gas-phase calculations only (Default)
NPHASE=2	Two-phase flash
NPHASE=3	Three-phase flash

3 ASME Power Test Code 10, (1965), pp. 31-32.

4 GPSA Engineering Data Book, (1979), pp. 5-6 to 5-10.

If you do not specify NPHASE, the default is to perform vapor phase calculations. At the end of calculations, the outlet stream is flashed at the outlet temperature and pressure to check for any condensation. If needed, the outlet stream is also checked at the outlet pressure and the intermediate isentropic temperature. If the vapor fraction calculated by either flash is less than 1.0, COMPR generates a message recommending you specify NPHASE=2.

SB-MAXIT ..... Maximum iterations for entropy balance calculations. Use only when TYPE=ISENTROPIC, ASME-ISENTROPIC, or ASME-POLYTROPIC. (Default=30)

SB-TOL..... Tolerance for entropy balance calculations. Use only when TYPE=ISENTROPIC, ASME-POLYTROPIC, or ASME-ISENTROPIC. (Default=$1x10^{-4}$)

MAXIT..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

TOL..... Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

PS-FLASH..... For constant entropy flash calculations, determines which algorithm to use:

PS-FLASH=DIRECT	Use direct call to Flash
PS-FLASH=INDIRECT	Perform a series of PQ flashes until the specified entropy is obtained (Default)

INT-METHOD The integration method used in polytropic and positive displacement model calculations:

INT-METHOD=N-METHOD	Using a piecewise integration with the relationship of pv^n=constant (see Note 12.)
INT-METHOD=DIRECT	Using a direct piecewise integration (see Note 12.)

INT-STEP For the integration method, method used for determining pressure change in the integration steps:

INT-STEP=EQUAL-PRATIO	Equal pressure ratio is used.
INT-STEP=EQUAL-DELP	Equal pressure change is used.

PRAT-STEP Pressure ratio in each integration step when INT-STEP=EQUAL-PRATIO (Default=1.25).

PRAT-FINAL Pressure ratio in the last integration step when INT-STEP=EQUAL-PRATIO (Default=1.375).

INTERVALS Number of intervals in piecewise integration of work integral when INT-STEP=EQUAL-DELP (Default=5).

PLOSS-FACTOR Scaling factor for power loss

PLOSS-OFFSET Offset for power loss. Units of power loss are used.

PL-FLOW-UNIT Units of flow rate used in power loss curve. Default is global unit.

PLOSS-UNITS Units of power loss used in power loss curve. Default is global unit.

PL-SP-UNIT Units of shaft speed used in power loss curve. Default is global unit.

PERFOR-PARAM Use to enter optional parameters related to compressor performance curves and suction pressure-loss calculations.

SUCT-NOZ-DIA..... Diameter of suction nozzle. Use to calculate pressure drop across suction nozzle of compressor, using the equation in Note 4.

SUCT-K-FACT ..... K-factor (velocity head multiplier) for suction nozzle. Use to calculate pressure drop across suction nozzle of compressor, using the equation in Note 4.

GPSA-BASIS..... Use when TYPE=GPSA-ISENTROPIC or GPSA-POLYTROPIC[5]

GPSA-BASIS=SUCTION	Uses suction conditions in head equation (Default)
GPSA-BASIS=AVERAGE	Uses average of suction and discharge conditions in head equation

NCURVES ..... Number of compressor performance curves. If:

- A single curve is supplied, it can be used to rate a compressor at a given speed
- A reference shaft speed is known, Fan laws will be used to scale the performance
- Multiple curves are supplied, linear interpolation is performed between curves to find the performance at operating point
- A user subroutine is used to enter performance specifications, set NCURVES=1

EXTRAPOLATE..... Indicates whether to extrapolate performance curve(s) beyond surge and stonewall points:

EXTRAPOLATE=YES	Extrapolates (Default)
EXTRAPOLATE=NO	Does not extrapolate

CALC-SPEED..... Indicates whether compressor shaft speed is calculated or specified:

CALC-SPEED=NO	Specified by user (Default)
CALC-SPEED=YES	Calculated by Aspen Plus model

ACT-SH-SPEED..... Speed of compressor shaft

IMPELLER-DIA..... Diameter of the compressor's impeller

USER-CURVES..... Specifies the type of performance variable (in addition to efficiency) supplied by a user subroutine:

USER-CURVES=HEAD	Head
USER-CURVES= HEAD-COEF	Head coefficient
USER-CURVES=POWER	Power
USER-CURVES=PRES	Discharge pressure
USER-CURVES=PRATIO	Pressure ratio
USER-CURVES=DELP	Pressure drop

REF-SH-SPEED..... Reference speed of compressor shaft. Use when Fan laws are applied to determine compressor performance.

FANEXPH ..... Fan law exponent for head (Default=2.0)

FANEXPE..... Fan law exponent for efficiency (Default=1.0)

FANEXPP..... Fan law exponent for power (Default=3.0)

SPLINE-FIT..... Interpolation method for tabular data

SPLINE-FIT= HARWELL	Cubic spline fit using Harwell method

5 GPSA Engineering Data Book, (1979), pp. 5-6 to 5-10.

	SPLINE-FIT= HERMITE	Cubic spline fit using Hermite method (Default)
	SPLINE-FIT= LINEAR	Linear interpolation between successive points
OPT-DESIGN	Options for off-design adjustments.	
	OPT-DESIGN= NONE	No off design adjustment (Default)
	OPT-DESIGN= CORR-FACTOR	Use a power correction factor to account for deviation from design conditions (only allowed for power curves)
	OPT-DESIGN= CORR-FLOW	Use corrected flow rate for performance curves
	OPT-DESIGN= DIMENSIONLESS	Use quasi-dimensionless performance curves
CORR-FLOW	Options for corrected flow used in performance curves.	
	CORR-FLOW = TP	The flow rate is corrected by the ratio of $\text{Pressure}/\sqrt{\text{Temperature}}$ at inlet design and actual conditions (Default)
	CORR-FLOW = PV	The flow rate is corrected by the ratio of $\sqrt{\text{Pressure}/\text{molar volume}}$ at inlet design and actual conditions
CURVE-DIM	Options for performance curve dimensionless groups.	
	CURVE-DIM= QUASI	Use quasi-dimensionless groups (Default)
	CURVE-DIM= R-QUASI	Use quasi-dimensionless groups containing gas constant R
DEF-PRATIO	Definitions of pressure ratio.	
	DEF-PRATIO= POUT-OV-PIN	Outlet pressure divided by inlet pressure (Default)
	DEF-PRATIO= PIN-OV-POUT	Inlet pressure divided by outlet pressure
GEAR-RATIO	The gear ratio between the driver and the compressor (compressor speed/driver speed). Use GEAR-RATIO only if speed is available in the inlet work stream.	
PIN-DESIGN	Inlet pressure at design conditions	
TIN-DESIGN	Inlet temperature at design conditions	
PIN-UNITS	Units of inlet pressure used in quasi-dimensionless curves	
TIN-UNITS	Units of inlet temperature used in quasi-dimensionless curves	
GAS-CONST-UNIT	Units of gas constant used in quasi-dimensionless curves (when CURVE-DIM = R-QUASI)	
HEAD-FACTOR	Scaling factor applied to head values calculated from either tabular (HEAD-TABLE) or polynomial (HEAD-POLY) data (Default=1)	
HEAD-OFFSET	Offset for head developed. Units of HEAD-UNITS are used.	
HEAD-NPOINT	Maximum number of data points in a curve when head versus flow curves are specified in a table	
H-FLOW-VAR	Independent flow variable used in head versus flow curves:	
	H-FLOW-VAR=VOL-FLOW	Volume flow
	H-FLOW-VAR= MASS-FLOW	Mass flow
H-FLOW-UNIT	Units of the independent flow variable in head versus flow curves	
HEAD-UNITS	Units of head data in head versus flow curves	

HEAD-SP-UNIT..... Units of shaft speed used in head curve (HEAD-CORR sentence). Default is global unit.

ACTUAL-HEAD..... Indicates if the head specified in the HEAD-TABLE, HEAD-POLY, or HEAD-CORR sentence is actual or polytropic/isentropic.(See Note 5.)

ACTUAL-HEAD=NO	Head is polytropic/isentropic (Default)
ACTUAL-HEAD=YES	Head is actual

HEADC-FACTOR..... Scaling factor applied to head coefficient values calculated from either tabular (HEADC-TABLE) or polynomial (HEADC-POLY) data of performance curves (Default=1)

HEADC-OFFSET ..... Offset for head coefficient

HEADC-NPOINT..... Maximum number of data points in a curve when head coefficient versus flow curves are specified in a table

HC-FLOW-VAR..... Independent flow variable used in head coefficient versus flow curves:

H-FLOW-VAR= "VOL-FLOW/N"	Volume flow per shaft speed in RPM, or specific flow
H-FLOW-VAR= FLOW-COEFF	Flow coefficient

HC-FLOW-UNIT ..... Units of the independent flow variable in head coefficient versus flow curves

ACTUAL-HEADC..... Indicates if the head coefficient specified in the HEADC-TABLE or HEADC-POLY sentence is actual or polytropic/isentropic. (See Note 5.)

ACTUAL-HEADC=NO	Head coefficient is polytropic/isentropic (Default)
ACTUAL-HEADC=YES	Head coefficient is actual

POWER-FACTOR..... Scaling factor applied to power values calculated from either tabular (POWER-TABLE) or polynomial (POWER-POLY) data (Default=1)

POWER-OFFSET ..... Offset for power. Units of POWER-UNITS are used.

POWER-NPOINT..... Maximum number of data points in a curve when power versus flow curves are specified in a table

PW-FLOW-VAR..... Independent flow variable used in power versus flow curves:

PW-FLOW-VAR= VOL-FLOW	Volume flow
PW-FLOW-VAR= MASS-FLOW	Mass flow

PW-FLOW-UNIT ..... Units of the independent flow variable in power versus flow curves

POWER-UNITS ..... Units of power data in power versus flow curves

PRES-FACTOR ..... Scaling factor applied to discharge pressure values calculated from either tabular (PRES-TABLE) or polynomial (PRES-POLY) data (Default=1)

PRES-OFFSET Offset for discharge pressure. Units of PRES-UNITS are used except for gauge pressure.

PRES-NPOINT ..... Maximum number of data points in a curve when discharge pressure versus flow curves are specified in a table

P-FLOW-VAR..... Independent flow variable used in discharge pressure versus flow curves:

	P-FLOW-VAR=VOL-FLOW	Volume flow
	P-FLOW-VAR=MASS-FLOW	Mass flow
P-FLOW-UNIT	Units of the independent flow variable in discharge pressure versus flow curves	
PRES-UNITS	Units of pressure data in discharge pressure versus flow curves	
PRAT-FACTOR	Scaling factor applied to pressure ratio values calculated from either tabular (PRATIO-TABLE) or polynomial (PRATIO-POLY) data (Default=1)	
PRAT-OFFSET	Offset for pressure ratio.	
PRAT-NPOINT	Maximum number of data points in a curve when pressure ratio versus flow curves are specified in a table	
PR-FLOW-VAR	Independent flow variable used in pressure ratio versus flow curves:	
	PR-FLOW-VAR=VOL-FLOW	Volume flow
	PR-FLOW-VAR=MASS-FLOW	Mass flow
PR-FLOW-UNIT	Units of the independent flow variable in pressure ratio versus flow curves	
DELP-FACTOR	Scaling factor applied to pressure change values calculated from either tabular (DELP-TABLE) or polynomial (DELP-POLY) data (Default=1)	
DELP-OFFSET	Offset for pressure change. Units of DELP-UNITS are used.	
DELP-NPOINT	Maximum number of data points in a curve when pressure change versus flow curves are specified in a table	
DP-FLOW-VAR	Independent flow variable used in pressure change versus flow curves:	
	DP-FLOW-VAR=VOL-FLOW	Volume flow
	DP-FLOW-VAR=MASS-FLOW	Mass flow
DP-FLOW-UNIT	Units of the independent flow variable in pressure change versus flow curves	
DELP-UNITS	Units of pressure change data in pressure change versus flow curves	
EFF-FACTOR	Scaling factor applied to efficiency values calculated from either tabular (EFF-TABLE) or polynomial (EFF-POLY) data (Default=1)	
EFF-OFFSET	Offset for efficiency.	
EFF-NPOINT	Maximum number of data points in a curve when efficiency versus flow curves are specified in a table	
EF-FLOW-VAR	Independent flow variable used in efficiency versus flow curves:	
	EF-FLOW-VAR=VOL-FLOW	Volume flow
	EF-FLOW-VAR=MASS-FLOW	Mass flow
	EF-FLOW-VAR="VOL-FLOW/N"	Volume flow per shaft speed in RPM or specific speed

	EF-FLOW-VAR= FLOW-COEFF	Flow coefficient
	EF-FLOW-UNIT	Units of the independent flow variable in efficiency versus flow curves
	EFF-SP-UNIT	Units of shaft speed used in efficiency curve (EFF-CORR sentence). Default is global unit.
	SURGE-FACTOR	Scaling factor for surge volumetric flow rate.
	SURGE-OFFSET	Offset for surge volumetric flow rate. Units of SURGE-UNITS are used.
	SURGE-UNITS	Units of surge volumetric flow rate used in surge curve. Default is global unit.
	SG-SP-UNIT	Units of shaft speed used in surge curve. Default is global unit.

HEAD-TABLE

Use to enter values of head developed versus suction flow rate in a table. You must also specify HEAD-NPOINT, HEAD-UNITS, H-FLOW-VAR, and H-FLOW-UNIT in the PERFOR-PARAM sentence. When performance curves are entered in tabular form, the first point of the table is taken as surge and the last point as stonewall, for a given curve. (See Notes 6 and 7.)

curve	Curve number
point	Row number within a table
head	Head developed. The head can be polytropic, isentropic, or actual, depending on TYPE and ACTUAL-HEAD specifications. (See Note 5.)
flow	Suction flow rate (volumetric or mass)

HEAD-POLY

Use to enter polynomial coefficients to calculate head developed as a function of suction flow rate. You can enter surge and stonewall values. You must also specify H-FLOW-VAR and H-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 6.) The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Suction flow rate (volumetric or mass)

Y = Head developed

curve	Curve number
COEF1	First coefficient of head versus flow polynomial
COEF2	Second coefficient of head versus flow polynomial
COEF3	Third coefficient of head versus flow polynomial
COEF4	Fourth coefficient of head versus flow polynomial
SURGE	Suction flow rate value at which the compressor surges
STONEWALL	Suction flow rate value at which the compressor stonewalls

HEADC-TABLE

Use to enter values of head coefficient versus either suction flow rate per shaft speed in rpm or flow coefficient, in a table. You must also specify HEADC-NPOINT, HC-FLOW-VAR, and HC-FLOW-UNIT (if applicable) in the PERFOR-PARAM sentence. When performance curves are entered in tabular form, the first point of the table is taken as surge and the last point as stonewall, for a given curve.
(See Notes 6, 7, and 8.)

curve	Curve number
point	Row number within a table

head-coeff ..... Head coefficient. The value can be polytropic, isentropic, or actual, depending on TYPE and ACTUAL-HEADC specifications. (See Note 5.)

flow ..... Suction flow rate per shaft speed in rpm, or value of flow coefficient

HEADC-POLY

Use to enter polynomial coefficients to calculate head coefficient as a function of either suction flow rate per shaft speed in rpm or flow coefficient, in polynomial form. You must also specify HC-FLOW-VAR and HC-FLOW-UNIT (if applicable) in the PERFOR-PARAM sentence. (See Notes 6 and 8.) You can also enter surge and stonewall values. The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Volumetric flow rate per shaft speed in rpm or flow coefficient

Y = Head coefficient

curve ..... Curve number

COEF1 ..... First coefficient of head coefficient versus flow polynomial

COEF2 ..... Second coefficient of head coefficient versus flow polynomial

COEF3 ..... Third coefficient of head coefficient versus flow polynomial

COEF4 ..... Fourth coefficient of head coefficient versus flow polynomial

SURGE ..... Flow coefficient, or specific flow at which the compressor surges

STONEWALL ..... Flow coefficient, or specific flow at which the compressor stonewalls

POWER-TABLE

Use to enter values of power supplied versus suction flow rate in a table. You must also specify POWER-NPOINT, POWER-UNITS, PW-FLOW-VAR, and PW-FLOW-UNIT in the PERFOR-PARAM sentence. When performance curves are entered in tabular form, the first point of the table is taken as surge and the last point as stonewall, for a given curve. (See Notes 6 and 7.)

curve ..... Curve number

point ..... Row number within a table

power ..... Power supplied

flow ..... Suction flow rate (volumetric or mass)

POWER-POLY

Use to enter polynomial coefficients to calculate the power supplied as a function of suction flow rate. You must also specify POWER-UNITS, PW-FLOW-VAR, and PW-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 6.) You can enter surge and stonewall values. The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Suction flow rate (volumetric or mass)

Y = Power supplied

curve ..... Curve number

COEF1 ..... First coefficient of power versus flow polynomial

COEF2 ..... Second coefficient of power versus flow polynomial

COEF3 ..... Third coefficient of power versus flow polynomial

COEF4 ..... Fourth coefficient of power versus flow polynomial

SURGE..... Suction flow rate at which the compressor surges

STONEWALL..... Suction flow rate at which the compressor stonewalls

PRES-TABLE

Use to enter values of discharge pressure versus suction flow rate in a table. You must also specify PRES-NPOINT, PRES-UNITS, P-FLOW-VAR, and P-FLOW-UNIT in the PERFOR-PARAM sentence. When performance curves are entered in tabular form, the first point of the table is taken as surge and the last point as stonewall, for a given curve. (See Notes 6 and 7.)

curve ..... Curve number

point ..... Row number within a table

pres ..... Discharge pressure

flow ..... Suction flow rate (volumetric or mass)

PRES-POLY

Use to enter polynomial coefficients to calculate discharge pressure as a function of suction flow rate. You must also specify PRES-UNITS, P-FLOW-VAR, and P-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 6.) You can enter surge and stonewall values. The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Suction flow rate (volumetric or mass)

Y = Discharge pressure

curve ..... Curve number

COEF1 ..... First coefficient of pressure versus flow polynomial

COEF2 ..... Second coefficient of pressure versus flow polynomial

COEF3 ..... Third coefficient of pressure versus flow polynomial

COEF4 ..... Fourth coefficient of pressure versus flow polynomial

SURGE..... Suction flow rate at which the compressor surges

STONEWALL..... Suction flow rate at which the compressor stonewalls

PRATIO-TABLE

Use to enter pressure ratio (discharge pressure/suction pressure) versus suction flow rate in a table. You must also specify PRAT-NPOINT, PR-FLOW-VAR, and PR-FLOW-UNIT in the PERFOR-PARAM sentence. When performance curves are entered in tabular form, the first point of the table is taken as surge and the last point as stonewall, for a given curve. (See Notes 6 and 7.)

curve ..... Curve number

point ..... Row number within a table

pratio..... Pressure ratio

flow ..... Suction flow rate (volumetric or mass)

PRATIO-POLY

Use to enter polynomial coefficients to calculate pressure ratio (discharge pressure/suction pressure) as a function of suction flow rate. You must also specify PR-FLOW-VAR and PR-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 6.) You can enter surge and stonewall values. The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Suction flow rate (volumetric or mass)

Y = Pressure ratio

curve ..... Curve number

COEF1 ..... First coefficient of pratio versus flow polynomial

COEF2 ..... Second coefficient of pratio versus flow polynomial

COEF3 ..... Third coefficient of pratio versus flow polynomial

COEF4 ..... Fourth coefficient of pratio versus flow polynomial

SURGE..... Suction flow rate at which the compressor surges

STONEWALL..... Suction flow rate at which the compressor stonewalls

DELP-TABLE

Use to enter values of pressure change (discharge pressure/suction pressure) versus suction flow rate in a table. You must also specify DELP-NPOINT, DELP-UNITS, DP-FLOW-VAR, and DP-FLOW-UNIT in the PERFOR-PARAM sentence. When performance curves are entered in tabular form, the first point of the table is taken as surge and the last point as stonewall, for a given curve. (See Notes 6 and 7.)

curve ..... Curve number

point ..... Row number within a table

delp ..... Pressure change

flow ..... Suction flow rate (volumetric or mass)

DELP-POLY

Use to enter polynomial coefficients to calculate pressure change (discharge pressure-suction pressure) as a function of suction flow rate. You must also specify DELP-UNITS, DP-FLOW-VAR, and DP-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 6.) You can enter surge and stonewall values. The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Suction flow rate (volumetric or mass)

Y = Pressure change

curve ..... Curve number

COEF1 ..... First coefficient of delp versus flow polynomial

COEF2 ..... Second coefficient of delp versus flow polynomial

COEF3 ..... Third coefficient of delp versus flow polynomial

COEF4 ..... Fourth coefficient of delp versus flow polynomial

SURGE..... Suction flow rate at which the compressor surges

STONEWALL..... Suction flow rate at which the compressor stonewalls

EFF-TABLE

Use to enter values of efficiency versus suction flow rate in a table. You must also specify EFF-NPOINT, EF-FLOW-VAR, and EF-FLOW-UNIT in the PERFOR-PARAM sentence. When performance curves are entered in tabular form, the first point of the table is taken as surge and the last point as stonewall, for a given curve. (See Notes 6, 7 and 9.)

curve ..... Curve number

point ..... Row number within a table

eff..... Efficiency (either polytropic or isentropic, depending on TYPE)

flow ..... Suction flow rate (volumetric, mass, specific flow, or flow coefficient)

EFF-POLY

Use to enter polynomial coefficients to calculate efficiency as a function of suction flow rate. You must also specify EF-FLOW-VAR and EF-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 9.) The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Suction flow rate (volumetric, mass, specific flow, or flow coefficient)

Y = Efficiency

curve ..... Curve number

COEF1 ..... First coefficient of efficiency versus flow polynomial

COEF2 ..... Second coefficient of efficiency versus flow polynomial

COEF3 ..... Third coefficient of efficiency versus flow polynomial

COEF4 ..... Fourth coefficient of efficiency versus flow polynomial

SHAFT-SPEED

Use to enter compressor shaft speeds when multiple performance curves, at multiple shaft speeds, are available. (See Note 10.)

curve ..... Curve number

shaft-speed..... Shaft speed

MACH-NO

Use to enter Mach numbers when multiple performance curves, at multiple Mach numbers, are available. (See Note 11.)

curve ..... Curve number

mach-no ..... Mach number

HEAD-CORR

Use to enter polynomial coefficients to calculate head developed as a function of suction flow rate and shaft speed. You must also specify H-FLOW-VAR and H-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 6.) The polynomial used is:

$Y = coef1 + coef2*N + coef3*N^2 + coef4*X + coef5*X^2 + coef6*(X/N) + coef7*(X/N)^2 + coef8*X^4$

Where:

N = Shaft speed

X = Suction volumetric flow rate

Y = Head developed

COEF1 ..... First coefficient of head versus flow correlation

COEF2 ..... Second coefficient of head versus flow correlation

COEF3 ..... Third coefficient of head versus flow correlation

COEF4 ..... Fourth coefficient of head versus flow correlation

COEF5 ..... Fifth coefficient of head versus flow correlation

COEF6 ..... Sixth coefficient of head versus flow correlation

COEF7 ..... Seventh coefficient of head versus flow correlation

COEF8 ..... Eighth coefficient of head versus flow correlation

EFF-CORR

Use to enter polynomial coefficients to calculate efficiency as a function of suction flow rate and shaft speed. You must also specify EF-FLOW-VAR and EF-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 9.) EFF-CORR is allowed only if HEAD-CORR is specified. The polynomial used is:

$Y = coef1 + coef2*N + coef3*N^2 + coef4*X + coef5*X^2 + coef6*(X/N) + coef7*(X/N)^2 + coef8*X^4$

Where:

N = Shaft speed

X = Suction volumetric flow rate

Y = Efficiency

COEF1 ..... First coefficient of efficiency versus flow correlation

COEF2 ..... Second coefficient of efficiency versus flow correlation

COEF3 ..... Third coefficient of efficiency versus flow correlation

COEF4 ..... Fourth coefficient of efficiency versus flow correlation

COEF5 ..... Fifth coefficient of efficiency versus flow correlation

COEF6 ..... Sixth coefficient of efficiency versus flow correlation

COEF7 ..... Seventh coefficient of efficiency versus flow correlation

COEF8 ..... Eighth coefficient of efficiency versus flow correlation

SURGE-POLY

Use to enter polynomial coefficients to calculate surge volumetric flow rate as a function of shaft speed. You can specify SURGE-UNITS and SG-SP-UNIT in the PERFOR-PARAM sentence. SURGE-POLY is allowed only if HEAD-CORR is specified. The polynomial used is:

$Y = coef1 + coef2*N + coef3*N^2$

Where:

N = Shaft speed

Y = Surge volumetric flow rate

COEF1 ..... First coefficient of surge volumetric flow rate polynomial

COEF2 ..... Second coefficient of surge volumetric flow rate polynomial

COEF3 ..... Third coefficient of surge volumetric flow rate polynomial

PLOSS-POLY

Use to enter polynomial coefficients to calculate power loss as a function of suction flow rate and shaft speed. You can specify PLOSS-UNITS, PL-FLOW-UNIT, and PL-SP-UNIT in the PARAM sentence. (See Note 3.) The polynomial used is:

$Y = coef1 + coef2*XN^2 + coef3*(X*N)^2$

Where:

N = Shaft speed

X = Suction volumetric flow rate

Y = Power loss

COEF1 ..... First coefficient of power loss polynomial

COEF2 ..... Second coefficient of power loss polynomial

COEF3 ..... Third coefficient of power loss polynomial

SUBROUTINE

Use to specify user-supplied subroutine for calculating performance curves. You must specify the type of curve using the USER-CURVES keyword in the PERFOR-PARAM sentence. The user subroutine must also calculate efficiency, whenever it is used to calculate any other performance variable. See *Aspen Plus User Models*, Chapter 22, for information about writing user-supplied subroutines for performance curves.

CURVES..... Name of user-supplied FORTRAN subroutine for performance curve calculations

USER-VECS Use to define the length of arrays for user-supplied performance curve subroutines.

NINT..... Length of integer parameter array for the user-supplied performance curve subroutine

NREAL..... Length of real parameter array for the user-supplied performance curve subroutine

NIWORK ..... Length of integer workspace array for the user-supplied performance curve subroutine

NWORK..... Length of real parameter array for the user-supplied performance curve subroutine

INT Use to enter values for the integer parameter array of the user-supplied performance curve subroutine.

value-list ..... List of integer values

REAL Use to enter values for the real parameter array of the user-supplied performance curve subroutine.

value-list ..... List of real values

UTILITY Use to specify an optional utility to provide heating or cooling duty.

UTILITY-ID..... Utility ID.

Accessing Variables in COMPR

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for a COMPR block.

Block Input

Sentence	Variables	ID1	ID2
PARAM	PRES, DELP, PRATIO, POWER, TEMP, PEFF, SEFF, MEFF, CLFR, SB-MAXIT, SB-TOL, MAXIT, TOL, PLOSS-FACTOR, PLOSS-OFFSET, PRAT-STEP, PRAT-FINAL	—	—
PERFOR-PARAM	SUCT-NOZ-DIA, SUCT-K-FACT, ACT-SH-SPEED, IMPELLER-DIA, REF-SH-SPEED, FANEXPH, FANEXPE, FANEXPP, HEAD-FACTOR, HEAD-OFFSET, HEADC-FACTOR, HEADC-OFFSET, POWER-FACTOR, POWER-OFFSET, PRES-FACTOR, PRES-OFFSET, PRAT-FACTOR, PRAT-OFFSET, DELP-FACTOR, DELP-OFFSET, EFF-FACTOR, EFF-OFFSET, SURGE-FACTOR, SURGE-OFFSET, GEAR-RATIO, TIN-DESIGN, PIN-DESIGN	—	—
HEAD-TABLE	HEAD, FLOW	curve	point
HEAD-POLY	COEF1, COEF2, COEF3, COEF4, SURGE, STONEWALL	curve	—
HEADC-TABLE	HEAD-COEF, FLOW	curve	point
HEADC-POLY	COEF1, COEF2, COEF3, COEF4, SURGE, STONEWALL	curve	—
POWER-TABLE	POWER, FLOW	curve	point
POWER-POLY	COEF1, COEF2, COEF3, COEF4, SURGE, STONEWALL	curve	—
PRES-TABLE	PRES, FLOW	curve	point
PRES-POLY	COEF1, COEF2, COEF3, COEF4, SURGE, STONEWALL	curve	—
PRATIO-TABLE	PRATIO, FLOW	curve	point
PRATIO-POLY	COEF1, COEF2, COEF3, COEF4, SURGE, STONEWALL	curve	—
DELP-TABLE	DELP, FLOW	curve	point
DELP-POLY	COEF1, COEF2, COEF3, COEF4, SURGE, STONEWALL	curve	—
EFF-TABLE	EFFICIENCY, FLOW	curve	point
EFF-POLY	COEF1, COEF2, COEF3, COEF4	curve	—
SHAFT-SPEED	SHAFT-SPEED	curve	—
MACH-NO	MACH-NO	curve	—
HEAD-CORR	COEF1, COEF2, COEF3, COEF4, COEF5, COEF6, COEF7, COEF8	—	—
EFF-CORR	COEF1, COEF2, COEF3, COEF4, COEF5, COEF6, COEF7, COEF8	—	—
SURGE-POLY	COEF1, COEF2, COEF3	—	—
PLOSS-POLY	COEF1, COEF2, COEF3	—	—

Block Results

Description	Sentence	Variable
Indicated horsepower	RESULTS	IND-POWER
Brake horsepower	RESULTS	BRAKE-POWER
Net work	RESULTS	NET-WORK
Power loss	RESULTS	POWER-LOSS
Polytropic efficiency	RESULTS	PEFF-CALC
Volumetric efficiency	RESULTS	VEFF-CALC
Mechanical efficiency	RESULTS	MEFF-CALC
Isentropic temperature	RESULTS	ISENTR-TEMP
Ideal head developed	RESULTS	HEAD-CAL
Actual head developed	RESULTS	HEAD-ACT
Isentropic power requirement	RESULTS	ISEN-POWER
Outlet pressure	RESULTS	OUT-PRES-CAL
Outlet temperature	RESULTS	OUT-TEMP-CAL
Inlet heat capacity ratio	RESULTS	IN-CPR
Inlet volumetric flow rate	RESULTS	VFLOW-IN
Outlet volumetric flow rate	RESULTS	VFLOW-OUT
Inlet compressibility ratio	RESULTS	Z-IN
Outlet compressibility ratio	RESULTS	Z-OUT
Average isentropic volume exponent	RESULTS	EXP-V-ISEN
Average actual volume exponent	RESULTS	EXP-V-POLY
Average isentropic temperature exponent	RESULTS	EXP-T-ISEN
Average actual temperature exponent	RESULTS	EXP-T-POLY
Percent above surge	PERF-RESULTS	ABOVE-SURGE
Percent below stonewall	PERF-RESULTS	BELOW-SWALL
Surge volumetric flow rate	PERF-RESULTS	SURGE-VOLUME
Stonewall volumentric flow rate	PERF-RESULTS	SWALL-VOLUME
Calculated compressor shaft speed	PERF-RESULTS	SHAFT-SPEED
Specific shaft speed	PERF-RESULTS	SP-SPEED
Sonic velocity of gas at suction	PERF-RESULTS	SUCT-SONIC-V
Specific diameter	PERF-RESULTS	SP-DIAM
Head coefficient	PERF-RESULTS	HEAD-COEF
Flow coefficient	PERF-RESULTS	FLOW-COEF
Inlet Mach number	PERF-RESULTS	IN-MACH-NO
Rotor tip Mach number	PERF-RESULTS	RT-MACH-NO
Calculated power correction factor used in off-design adjustment	PERF-RESULTS	POWER-FACTOR
Specified or calculated gear ratio between the driver and the compressor	PERF-RESULTS	GEAR-RATIO-C

MCOMPR: Multistage Compressor/Turbine

Input Language for MCOMPR

```
BLOCK    blockid    MCOMPR
PARAM    keyword=value
```

Keywords:

NSTAGE TYPE

Optional keywords:

PRES COMPR-NPHASE COOLER-NPHASE TEMP-MAXIT TEMP-TOL SB-MAXIT SB-TOL MAXIT TOL PS-FLASH

```
FEEDS    sid    stage / . . .
PRODUCTS    sid    stage    [phase] / . . .
COMPR-SPECS    stage    keyword=value / . . .
```

Keywords:

PRES DELP PRATIO POWER TEMP

Optional keywords:

PEFF SEFF MEFF CLFR

```
COOLER-SPECS    stage    keyword=value / . . .
```

Keywords:

TRATIO TEMP DUTY

Optional keyword:

PDROP

```
PERFOR-PARAM    keyword=value
```

Optional keywords:

GPSA-BASIS NCURVES EXTRAPOLATE CALC-SPEED USER-CURVES NMAP
MAX-NWHEEL ACTUAL-HEAD ACTUAL-HEADC

Optional keywords for head curves:

HEAD-FACTOR HEAD-NPOINT H-FLOW-VAR H-FLOW-UNIT HEAD-UNITS ACTUAL-HEAD

Optional keywords for head coefficient curves:

HEADC-FACTOR HEADC-NPOINT HC-FLOW-VAR HC-FLOW-UNIT ACTUAL-HEADC

Optional keywords for power curves:

POWER-FACTOR POWER-NPOINT PW-FLOW-VAR PW-FLOW-UNIT POWER-UNITS

Optional keywords for discharge pressure curves:

PRES-FACTOR PRES-NPOINT P-FLOW-VAR P-FLOW-UNIT PRES-UNITS

Optional keywords for pressure ratio curves:

PRAT-FACTOR PRAT-NPOINT PR-FLOW-VAR PR-FLOW-UNIT

Optional keywords for pressure change curves:

DELP-FACTOR DELP-NPOINT DP-FLOW-VAR DP-FLOW-UNIT DELP-UNITS

Optional keywords for efficiency curves:

EFF-FACTOR EFF-NPOINT EF-FLOW-VAR EF-FLOW-UNIT

HEAD-TABLE map curve point head flow / ....
HEAD-POLY map curve *keyword=value* **/ ...**

Keywords:

COEF1 COEF2 COEF3 COEF4 SURGE STONEWALL

HEADC-TABLE map curve point head-coeff flow / ...
HEADC-POLY map curve *keyword=value* **/ ...**

Keywords:

COEF1 COEF2 COEF3 COEF4 SURGE STONEWALL

POWER-TABLE map curve point power flow / ....
POWER-POLY map curve *keyword=value* **/ ...**

Keywords:

COEF1 COEF2 COEF3 COEF4 SURGE STONEWALL

PRES-TABLE map curve point pres flow / ....
PRES-POLY map curve *keyword=value* **/ ...**

Keywords:

COEF1 COEF2 COEF3 COEF4 SURGE STONEWALL

PRATIO-TABLE map curve point pratio flow / ....
PRATIO-POLY map curve *keyword=value* **/ ...**

Keywords:

COEF1 COEF2 COEF3 COEF4 SURGE STONEWALL

DELP-TABLE map curve point delp flow / ....
DELP-POLY map curve *keyword=value* **/ ...**

Keywords:

COEF1 COEF2 COEF3 COEF4 SURGE STONEWALL

EFF-TABLE map curve point eff flow / ....
EFF-POLY map curve *keyword=value* **/ ...**

Keywords:

COEF1 COEF2 COEF3 COEF4

STAGE-DATA **stage** *keyword=value*

Keywords:

SUCT-NOZ-DIA SUCT-K-FACT ACT-SH-SPEED REF-SH-SPEED FANEXPH FANEXPE FANEXPP NWHEELS MAP SCL-FACTOR1 SCL-FACTOR2

WHEEL-DATA **stage** **wheel** *keyword=value* **/ ...**

Keywords:

FANEXPH FANEXPE FANEXPP IMPELLER-DIA MAP SCL-FACTOR1 SCL-FACTOR2

SHAFT-SPEED map curve shaft-speed / ...
MACH-NO map curve mach-no / ...
SUBROUTINE CURVES=subrname
USER-VECS *keyword=value*

Optional keywords:

NINT NREAL NIWORK NWORK

INT value-list
REAL value-list
HCURVE curveno stage *keyword=value*

Optional keywords:

INDEP-VAR LIST NPOINT INCR HEADING PROPERTIES PRES-PROFILE
PDROP PRINT-PLOT HIGH-PRECISION LINES X-SCALE Y-SCALE WIDE
GRID INTERPOLATE

Input Language Description for MCOMPR

PARAM Use to specify compressor type, number of stages, outlet pressure of the last stage of the compressor, and optional convergence parameters.

NSTAGE.....	Number of compression stages	
TYPE	**TYPE=ISENTROPIC**	Isentropic compressor/turbine
	TYPE=POS-DISP	Polytropic positive-displacement compressor calculations
	TYPE= ASME-POLYTROPIC	Polytropic compressor calculations using the ASME method[6]
	TYPE=ASME-ISENTROPIC	Isentropic compressor calculations using the ASME method[6]
	TYPE= GPSA-POLYTROPIC	Polytropic compressor calculations using the GPSA method[7]
	TYPE=GPSA-ISENTROPIC	Isentropic compressor calculations using the GPSA method[7]
PRES.....	Outlet pressure of the compressor	

6 ASME Power Test Code 10, (1965), pp. 31-32.

7 GPSA Engineering Data Book, (1979), pp. 5-6 to 5-10.

COMPR-NPHASE..... **COMPR-NPHASE=1** Gas-phase calculations only (Default)

COMPR-NPHASE=2 Two-phase flash

If you do not specify COMPR-NPHASE, the default is to perform vapor phase calculations. At the end of calculations, the outlet stream is flashed at the outlet temperature and pressure to check for any condensation. If needed, the outlet stream is also flashed at outlet pressure and the intermediate isentropic temperature. If the vapor fraction calculated by either flash is less than 1.0, MCOMPR generates a message recommending that you specify COMPR-NPHASE=2.

COOLER-NPHASE ..... Cooler calculations:

COOLER-NPHASE=1 Gas-phase calculations only

COOLER-NPHASE=2 Two-phase flash (Default)

COOLER-NPHASE=3 Three-phase flash

TEMP-MAXIT ..... Maximum iterations for temperature loop convergence. Use only when TEMP is specified using COMPR-SPECS. (Default=30)

TEMP-TOL ..... Tolerance for temperature loop convergence. Use only when TEMP is specified using COMPR-SPEC. (Default=0.01 K)

SB-MAXIT ..... Maximum iterations for entropy balance calculations. Use only when TYPE=ISENTROPIC, ASME-POLYTROPIC, or ASME-ISENTROPIC. (Default=30)

SB-TOL..... Tolerance for entropy balance calculations. Use only when TYPE=ISENTROPIC, ASME-POLYTROPIC, or ASME-ISENTROPIC. (Default=$1x10^{-4}$)

MAXIT..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

TOL ..... Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

PS-FLASH..... For constant entropy flash calculations, determines which algorithm to use:

PS-FLASH=DIRECT Use direct call to Flash

PS-FLASH=INDIRECT Perform a series of PQ flashes until the specified entropy is obtained (Default)

FEEDS

Use to enter feed stage locations for all inlet streams. There must be at least one inlet material stream to *stage1*. Any other inlet streams are optional. An inlet material stream to any stage other than *stage1* actually enters the preceding cooler. Any number of heat streams, work streams, and material streams can enter any stage.

sid..... Stream ID

stage..... Stage number

PRODUCTS

Use to enter stage locations for all outlet streams, including heat and work streams. A stage number entry of GLOBAL indicates the stream is a heat, work, or liquid GLOBAL outlet applying to all stages. For material streams, a stage number of 1, . . ., NSTAGE – 1 indicates a liquid knockout or water decant stream. A stage number of NSTAGE indicates the required compressor outlet stream.

sid..... Stream ID

stage..... Stage number or GLOBAL

phase..... Phase for liquid knockout and water decant streams:

L Total liquid (Default)

L1	Organic liquid
W	Free-water

If water or organic liquid is decanted, then both L1 and W phase product streams must be present.

COMPR-SPECS

Use to specify PRATIO, PRES, DELP, TEMP, or POWER for each stage of the compressor, if you do not:

- Specify the outlet pressure in the PARAM sentence
- Enter performance curves

The specification type must be the same for all stages. If you give both TEMP and a pressure specification, MCOMPR uses TEMP as an upper limit on temperature. You can use inlet work streams in place of COMPR-SPECS power specifications. If you do not specify all stages, the missing specifications default to the previous stage values. You can also use COMPR-SPECS to enter efficiencies.

stage	Stage number
PRES	Outlet pressure for the stage
DELP	Pressure change for the stage
PRATIO	Pressure ratio per stage
POWER	Power input to the stage. Power supplied to the stage is positive. Work streams use the opposite convention.
TEMP	Temperature at the outlet of the compression stage
PEFF	Polytropic efficiency as defined in Note 1. Use only when TYPE=ASME-POLYTROPIC, GPSA-POLYTROPIC, or POS-DISP. (Default=0.72)
SEFF	Isentropic efficiency as defined in Note 2. Use only when TYPE=ISENTROPIC, ASME-ISENTROPIC, or GPSA-ISENTROPIC. (Default=0.72)
MEFF	Mechanical efficiency as defined in Note 3. (Default=1)
CLFR	Clearance fraction. Use only when TYPE=POS-DISP. (Default=0.5)

COOLER-SPECS

Use to enter cooler specifications. There is an intercooler between each compression stage and an aftercooler following the last compression stage. For each cooler you must specify: TRATIO, TEMP, or DUTY. You can use inlet heat streams in place of COOLER-SPECS specifications. If no aftercooler is present, you must specify DUTY=0 for stage NSTAGE. If you do not specify all stages, the missing specifications default to previous stage values.

stage	Stage number
TRATIO	Ratio of the outlet temperature to the inlet temperature of the cooler
TEMP	Outlet temperature of the cooler
DUTY	Cooler heat duty. Negative for heat removal.
PDROP	Pressure drop across the cooler (Default=0)

PERFOR-PARAM

Use to enter optional parameters related to compressor performance curves and suction pressure-loss calculations.

GPSA-BASIS	Use when TYPE=GPSA-ISENTROPIC or GPSA-POLYTROPIC[8]

8 GPSA Engineering Data Book, (1979), pp. 5-6 to 5-10.

	GPSA-BASIS=SUCTION	Uses suction conditions in head equation (Default)
	GPSA-BASIS=AVERAGE	Uses average of suction and discharge conditions in head equation

NCURVES ..... Number of compressor performance curves. If:

- A single curve is supplied, it can be used to rate a compressor at a given speed
- A reference shaft speed is known, Fan laws will be used to scale the performance
- Multiple curves are supplied, linear interpolation is performed between curves to find the performance at operating point
- A user subroutine is used to enter performance specifications, set NCURVES=1

EXTRAPOLATE..... Indicates whether to extrapolate performance curve(s) beyond surge and stonewall points:

EXTRAPOLATE=YES	Extrapolates (Default)
EXTRAPOLATE=NO	Does not extrapolate

CALC-SPEED..... Indicates whether compressor shaft speed is calculated or specified:

CALC-SPEED=NO	Specified by user (Default)
CALC-SPEED=YES	Calculated by Aspen Plus model

USER-CURVES ..... Specifies the type of performance variable (in addition to efficiency) supplied by a user subroutine:

USER-CURVES=HEAD	Head
USER-CURVES= HEAD-COEF	Head coefficient
USER-CURVES=POWER	Power
USER-CURVES=PRES	Discharge pressure
USER-CURVES=PRATIO	Pressure ratio
USER-CURVES=DELP	Pressure drop

NMAP..... Number of performance maps

MAX-NWHEEL ..... Maximum number of wheels in any given stage

ACTUAL-HEAD..... Indicates if the head specified in the HEAD-TABLE or HEAD-POLY sentence is actual or polytropic/isentropic. (See Note 5.)

ACTUAL-HEAD=NO	Head is polytropic/isentropic (Default)
ACTUAL-HEAD=YES	Head is actual

ACTUAL-HEADC..... Indicates if the head coefficient specified in the HEADC-TABLE or HEADC-POLY sentence is actual or polytropic/isentropic. (See Note 5.)

ACTUAL-HEADC=NO	Head coefficient is polytropic/isentropic (Default)
ACTUAL-HEADC=YES	Head coefficient is actual

HEAD-FACTOR..... Scaling factor applied to head values calculated from either tabular (HEAD-TABLE) or polynomial (HEAD-POLY) data (Default=1)

HEAD-NPOINT..... Maximum number of data points in a curve when head versus flow curves are specified in a table

H-FLOW-VAR..... Independent flow variable used in head versus flow curves:

H-FLOW-VAR=VOL-FLOW	Volume flow
H-FLOW-VAR= MASS-FLOW	Mass flow

H-FLOW-UNIT ..... Units of the independent flow variable in head versus flow curves

HEAD-UNITS ..... Units of head data in head versus flow curves

HEADC-FACTOR..... Scaling factor applied to head coefficient values calculated from either tabular (HEADC-TABLE) or polynomial (HEADC-POLY) data (Default=1)

HEADC-NPOINT..... Maximum number of data points in a curve when head coefficient versus flow curves are specified in a table

HC-FLOW-VAR..... Independent flow variable used in head coefficient versus flow curves:

H-FLOW-VAR= "VOL-FLOW/N"	Volume flow per shaft speed in RPM, or specific flow rate
H-FLOW-VAR= FLOW-COEFF	Flow coefficient

HC-FLOW-UNIT ..... Units of the independent flow variable in head coefficient versus flow curves

POWER-FACTOR..... Scaling factor applied to power values calculated from either tabular (POWER-TABLE) or polynomial (POWER-POLY) data (Default=1)

POWER-NPOINT..... Maximum number of data points in a curve when power versus flow curves are specified in a table

PW-FLOW-VAR..... Independent flow variable used in power versus flow curves:

PW-FLOW-VAR= VOL-FLOW	Volume flow
PW-FLOW-VAR= MASS-FLOW	Mass flow

PW-FLOW-UNIT ..... Units of the independent flow variable in power versus flow curves

POWER-UNITS ..... Units of power data in power versus flow curves

PRES-FACTOR ..... Scaling factor applied to discharge pressure values calculated from either tabular (PRES-TABLE) or polynomial (PRES-POLY) data (Default=1)

PRES-NPOINT ..... Maximum number of data points in a curve when discharge pressure versus flow curves are specified in a table

P-FLOW-VAR..... Independent flow variable used in discharge pressure versus flow curves:

P-FLOW-VAR= VOL-FLOW	Volume flow
P-FLOW-VAR= MASS-FLOW	Mass flow

P-FLOW-UNIT ..... Units of the independent flow variable in discharge pressure versus flow curves

PRES-UNITS..... Units of pressure data in pressure versus flow curves

PRAT-FACTOR ..... Scaling factor applied to pressure ratio values calculated from either tabular (PRATIO-TABLE) or polynomial (PRATIO-POLY) data (Default=1)

PRAT-NPOINT ..... Maximum number of data points in a curve when pressure ratio versus flow curves are specified in a table

PR-FLOW-VAR..... Independent flow variable used in pressure ratio versus flow curves:

	PR-FLOW-VAR= VOL-FLOW	Volume flow
	PR-FLOW-VAR= MASS-FLOW	Mass flow

PR-FLOW-UNIT ..... Units of the independent flow variable in pressure ratio versus flow curves

DELP-FACTOR ..... Scaling factor applied to pressure change values calculated from either tabular (DELP-TABLE) or polynomial (DELP-POLY) data (Default=1)

DELP-NPOINT ..... Maximum number of data points in a curve when pressure change versus flow curves are specified in a table

DP-FLOW-VAR..... Independent flow variable used in pressure change versus flow curves:

DP-FLOW-VAR= VOL-FLOW	Volume flow
DP-FLOW-VAR= MASS-FLOW	Mass flow

DP-FLOW-UNIT ..... Units of the independent flow variable in pressure change versus flow curves

DELP-UNITS..... Units of pressure change data in pressure change versus flow curves

EFF-FACTOR..... Scaling factor applied to efficiency values calculated from either tabular (EFF-TABLE) or polynomial (EFF-POLY) data (Default=1)

EFF-NPOINT..... Maximum number of data points in a curve when efficiency versus flow curves are specified in a table

EF-FLOW-VAR ..... Independent flow variable used in efficiency versus flow curves:

EF-FLOW-VAR= VOL-FLOW	Volume flow
EF-FLOW-VAR= MASS-FLOW	Mass flow
EF-FLOW-VAR= "VOL-FLOW/N"	Volume flow per shaft speed in RPM, or specific flow
EF-FLOW-VAR= FLOW-COEFF	Flow coefficient

EF-FLOW-UNIT..... Units of the independent flow variable in efficiency versus flow curves

HEAD-TABLE Use to enter values of head developed versus suction flow rate in a table. You must also specify HEAD-NPOINT, HEAD-UNITS, H-FLOW-VAR, and H-FLOW-UNIT in the PERFOR-PARAM sentence. When performance curves are entered in tabular form, the first point of the table is taken as surge and the last point as stonewall, for a given curve. (See Notes 6 and 7.)

map ..... Map number

curve ..... Curve number

point..... Row number within a table

head ..... Head developed. The head can be polytropic, isentropic, or actual, depending on TYPE and ACTUAL-HEAD specifications. (See Note 5.)

flow ..... Suction flow rate (volumetric or mass)

HEAD-POLY

Use to enter polynomial coefficients to calculate head developed as a function of suction flow rate. You must also specify HEAD-UNITS, H-FLOW-VAR, and H-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 6.) You can enter surge and stonewall values. The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Suction flow rate (volumetric or mass)

Y = Head developed

map ..... Map number

curve ..... Curve number

COEF1 ..... First coefficient of head versus flow polynomial

COEF2 ..... Second coefficient of head versus flow polynomial

COEF3 ..... Third coefficient of head versus flow polynomial

COEF4 ..... Fourth coefficient of head versus flow polynomial

SURGE..... Suction flow rate value at which the compressor surges

STONEWALL..... Suction flow rate value at which the compressor stonewalls

HEADC-TABLE

Use to enter values of head coefficient versus either suction flow rate per shaft speed in rpm or flow coefficient, in a table. You must also specify HEADC-NPOINT, HC-FLOW-VAR, and HC-FLOW-UNIT (if applicable) in the PERFOR-PARAM sentence. When performance curves are entered in tabular form, the first point of the table is taken as surge and the last point as stonewall, for a given curve.
(See Notes 6, 7, and 8.)

map ..... Map number

curve ..... Curve number

point ..... Row number within a table

head-coeff ..... Head coefficient. The value can be polytropic, isentropic, or actual, depending on TYPE and ACTUAL-HEADC specifications. (See Note 5.)

flow ..... Suction flow rate per shaft speed in rpm, or flow coefficient

HEADC-POLY

Use to enter polynomial coefficients to calculate head coefficient as a function of either suction flow rate per shaft speed in rpm or flow coefficient, in polynomial form. You must also specify HC-FLOW-VAR and HC-FLOW-UNIT (if applicable) in the PERFOR-PARAM sentence. (See Notes 6 and 8.) You can enter surge and stonewall values. The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Volumetric flow rate per shaft speed in rpm, or flow coefficient

Y = Head coefficient

map ..... Map number

curve ..... Curve number

COEF1 ..... First coefficient of head coefficient versus flow polynomial

COEF2 ..... Second coefficient of head coefficient versus flow polynomial

COEF3 ..... Third coefficient of head coefficient versus flow polynomial

COEF4 ..... Fourth coefficient of head coefficient versus flow polynomial

SURGE..... Flow coefficient, or specific flow at which the compressor surges

STONEWALL..... Flow coefficient, or specific flow at which the compressor stonewalls

POWER-TABLE

Use to enter values of power supplied versus suction flow rate in a table. You must also specify POWER-NPOINT, POWER-UNITS, PW-FLOW-VAR, and PW-FLOW-UNIT in the PERFOR-PARAM sentence. When performance curves are entered in tabular form, the first point of the table is taken as surge and the last point as stonewall, for a given curve. (See Notes 6 and 7.)

map ..... Map number

curve ..... Curve number

point ..... Row number within a table

power ..... Power supplied

flow ..... Suction flow rate (volumetric or mass)

POWER-POLY

Use to enter polynomial coefficients to calculate power supplied as a function of suction flow rate. You must also specify POWER-UNITS, PW-FLOW-VAR, and PW-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 6.) You can enter surge and stonewall values. The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Suction flow rate (volumetric or mass)

Y = Power supplied

map ..... Map number

curve ..... Curve number

COEF1 ..... First coefficient of power versus flow polynomial

COEF2 ..... Second coefficient of power versus flow polynomial

COEF3 ..... Third coefficient of power versus flow polynomial

COEF4 ..... Fourth coefficient of power versus flow polynomial

SURGE..... Suction flow rate at which the compressor surges

STONEWALL..... Suction flow rate at which the compressor stonewalls

PRES-TABLE

Use to enter values of discharge pressure versus suction flow rate in a table. You must also specify PRES-NPOINT, PRES-UNITS, P-FLOW-VAR, and P-FLOW-UNIT in the PERFOR-PARAM sentence. When performance curves are entered in tabular form, the first point of the table is taken as surge and the last point as stonewall, for a given curve. (See Notes 6 and 7.)

map ..... Map number

curve ..... Curve number

point ..... Row number within a table

pres ..... Discharge pressure

flow ..... Suction flow rate (volumetric or mass)

PRES-POLY

Use to enter polynomial coefficients to calculate discharge pressure as a function of suction flow rate. You must also specify PRES-UNITS, P-FLOW-VAR, and P-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 6.) You can enter surge and stonewall values. The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Suction flow rate (volumetric or mass)

Y = Discharge pressure

map ..... Map number

curve ..... Curve number

COEF1 ..... First coefficient of pressure versus flow polynomial

COEF2 ..... Second coefficient of pressure versus flow polynomial

COEF3 ..... Third coefficient of pressure versus flow polynomial

COEF4 ..... Fourth coefficient of pressure versus flow polynomial

SURGE..... Suction flow rate at which the compressor surges

STONEWALL..... Suction flow rate at which the compressor stonewalls

PRATIO-TABLE

Use to enter values of pressure ratio (discharge pressure/suction pressure) versus suction flow rate in a table. You must also specify PRAT-NPOINT, PR-FLOW-VAR, and PR-FLOW-UNIT in the PERFOR-PARAM sentence. When performance curves are entered in tabular form, the first point of the table is taken as surge and the last point as stonewall, for a given curve. (See Notes 6 and 7.)

map ..... Map number

curve ..... Curve number

point ..... Row number within a table

pratio..... Pressure ratio

flow ..... Suction flow rate (volumetric or mass)

PRATIO-POLY

Use to enter polynomial coefficients to calculate pressure ratio (discharge pressure/suction pressure) as a function of suction flow rate. You must also specify PR-FLOW-VAR and PR-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 6.) You can enter surge and stonewall values. The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Suction flow rate (volumetric or mass)

Y = Pressure ratio

map ..... Map number

curve ..... Curve number

COEF1 ..... First coefficient of pratio versus flow polynomial

COEF2 ..... Second coefficient of pratio versus flow polynomial

COEF3 ..... Third coefficient of pratio versus flow polynomial

COEF4 ..... Fourth coefficient of pratio versus flow polynomial

SURGE..... Suction flow rate at which the compressor surges

STONEWALL ..... Suction flow rate at which the compressor stonewalls

DELP-TABLE

Use to enter values of pressure change (discharge pressure-suction pressure) versus suction flow rate in a table. You must also specify DELP-NPOINT, DELP-UNITS, DP-FLOW-VAR, and DP-FLOW-UNIT in the PERFOR-PARAM sentence. When performance curves are entered in tabular form, the first point of the table is taken as surge and the last point as stonewall, for a given curve. (See Notes 6 and 7.)

map ..... Map number

curve ..... Curve number

point ..... Row number within a table

delp ..... Pressure change

flow ..... Suction flow rate (volumetric or mass)

DELP-POLY

Use to enter polynomial coefficients to calculate pressure change (discharge pressure-suction pressure) as a function of suction flow rate. You must also specify DELP-UNITS, DP-FLOW-VAR, and DP-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 6.) You can enter surge and stonewall values. The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Suction flow rate (volumetric or mass)

Y = Pressure change

map ..... Map number

curve ..... Curve number

COEF1 ..... First coefficient of delp versus flow polynomial

COEF2 ..... Second coefficient of delp versus flow polynomial

COEF3 ..... Third coefficient of delp versus flow polynomial

COEF4 ..... Fourth coefficient of delp versus flow polynomial

SURGE ..... Suction flow rate at which the compressor surges

STONEWALL ..... Suction flow rate at which the compressor stonewalls

EFF-TABLE

Use to enter values of efficiency versus suction flow rate in a table. You must also specify EFF-NPOINT, EF-FLOW-VAR, and EF-FLOW-UNIT in the PERFOR-PARAM sentence. When performance curves are entered in tabular form, the first point of the table is taken as surge and the last point as stonewall, for a given curve. (See Notes 6, 7 and 9.)

map ..... Map number

curve ..... Curve number

point ..... Row number within a table

eff ..... Efficiency (either polytropic or isentropic, depending on TYPE)

flow ..... Suction flow rate (volumetric, mass, specific flow, or flow coefficient)

EFF-POLY

Use to enter polynomial coefficients to calculate efficiency as a function of suction flow rate. You must also specify EF-FLOW-VAR and EF-FLOW-UNIT in the PERFOR-PARAM sentence. (See Note 6.) The polynomial used is:

$Y = coef1 + coef2*X + coef3*X^2 + coef4*X^3$

Where:

X = Suction flow rate (volumetric, mass, specific flow, or flow coefficient)

Y = Efficiency

map ..... Map number

curve ..... Curve number

COEF1 ..... First coefficient of efficiency versus flow polynomial

COEF2 ..... Second coefficient of efficiency versus flow polynomial

COEF3 ..... Third coefficient of efficiency versus flow polynomial

COEF4 ..... Fourth coefficient of efficiency versus flow polynomial

STAGE-DATA

Use to enter any stage-specific performance parameters.

stage..... Stage number

SUCT-NOZ-DIA..... Diameter of suction nozzle for a stage. This value is used to calculate pressure drop across the suction nozzle of a compressor stage, using the equation in Note 4.

SUCT-K-FACT ..... K-factor (velocity head multiplier) of suction nozzle for a stage. This value is used to calculate pressure drop across the suction nozzle of a compressor stage, using the equation in Note 4.

ACT-SH-SPEED ..... Speed of compressor shaft at a given stage

REF-SH-SPEED ..... Reference speed of compressor shaft at a given stage. Use when Fan laws are applied to determine compressor performance.

FANEXPH ..... Fan law exponent for head (Default=2.0)

FANEXPE..... Fan law exponent for efficiency (Default=1.0)

FANEXPP..... Fan law exponent for power (Default=3.0)

NWHEELS..... Number of wheels in a stage

MAP ..... Performance map number associated with this stage

SCL-FACTOR1..... Scale factor used to multiply the performance variable calculated for a stage. The performance variable is calculated from one of the following performance curves: head, head coefficient, power, pres, pratio, or delp.

SCL-FACTOR2..... Scale factor used to multiply the stage efficiency value calculated from performance curves

WHEEL-DATA

Use to enter wheel-specific performance parameters when you enter wheel-by-wheel performance curves.

stage..... Stage number

wheel..... Wheel number

FANEXPH ..... Fan law exponent for head (Default=2.0)

FANEXPE..... Fan law exponent for efficiency (Default=1.0)

FANEXPP..... Fan law exponent for power (Default=3.0)

IMPELLER-DIA ..... Diameter of the compressor's impeller

MAP ..... Performance map number associated with this wheel

SCL-FACTOR1..... Scale factor used to multiply the performance variable calculated for a wheel. The performance variable is calculated from one of the following performance curves: head, head coefficient, power, pres, pratio, or delp.

SCL-FACTOR2..... Scale factor used to multiply the wheel efficiency value calculated from performance curves

SHAFT-SPEED Use to enter compressor shaft speeds when multiple performance curves, at multiple shaft speeds, are available. (See Note 10.)

map ..... Map number

curve ..... Curve number

shaft-speed..... Shaft speed

MACH-NO Use to enter Mach numbers when multiple performance curves, at multiple Mach numbers, are available. (See Note 11.)

map ..... Map number

curve ..... Curve number

mach-no ..... Mach number

SUBROUTINE Use to specify user-supplied subroutine for calculating performance curves. You must specify the type of curve using the USER-CURVES keyword in the PERFOR-PARAM sentence. The user subroutine must also calculate efficiency, whenever it is used to calculate any other performance variable. See *Aspen Plus User Models*, Chapter 22, for information about writing user-supplied subroutines for performance curves.

CURVES..... Name of user-supplied FORTRAN subroutine for performance curve calculations

USER-VECS Use to define the length of arrays for user-supplied performance curve subroutines.

NINT..... Length of integer parameter array for the user-supplied performance curve subroutine

NREAL..... Length of real parameter array for the user-supplied performance curve subroutine

NIWORK ..... Length of integer workspace array for the user-supplied performance curve subroutine

NWORK..... Length of real parameter array for the user-supplied performance curve subroutine

INT Use to enter values for the integer parameter array of the user-supplied performance curve subroutine.

value-list ..... List of integer values

REAL Use to enter values for the real parameter array of the user-supplied performance curve subroutine.

value-list ..... List of real values

HCURVE Use to generate heating or cooling curve tables and plots for the turbine or compressor. You must specify stage number. See Chapter 11 for a description of the input keywords.

stage..... Stage number

Accessing Variables in MCOMPR

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for an MCOMPR block.

Block Input

Sentence	Variables	ID1	ID2	ID3
PARAM	NSTAGE, PRES, TEMP-MAXIT, TEMP-TOL, SB-MAXIT, SB-TOL, MAXIT, TOL	—	—	—
COMPR-SPECS	PRES, DELP, PRATIO, POWER, PEFF, SEFF, MEFF, CLFR, TEMP	stage	—	—
COOLER-SPECS	TRATIO, TEMP, DUTY, PDROP	stage	—	—
FEEDS	STAGE	sid	—	—
PRODUCTS	STAGE	sid	—	—
HEAD-TABLE	HEAD, FLOW	map	curve	point
HEAD-POLY	COEF1, COEF2, COEF3, COEF4, SURGE, STONEWALL	map	curve	—
HEADC-TABLE	HEAD-COEF, FLOW	map	curve	point
HEADC-POLY	COEF1, COEF2, COEF3, COEF4, SURGE, STONEWALL	map	curve	—
POWER-TABLE	POWER, FLOW	map	curve	point
POWER-POLY	COEF1, COEF2, COEF3, COEF4, SURGE, STONEWALL	map	curve	—
PRES-TABLE	PRES, FLOW	map	curve	point
PRES-POLY	COEF1, COEF2, COEF3, COEF4, SURGE, STONEWALL	map	curve	—
PRATIO-TABLE	PRATIO, FLOW	map	curve	point
PRATIO-POLY	COEF1, COEF2, COEF3, COEF4, SURGE, STONEWALL	map	curve	—
DELP-TABLE	DELP, FLOW	map	curve	point
DELP-POLY	COEF1, COEF2, COEF3, COEF4, SURGE, STONEWALL	map	curve	—
EFF-TABLE	EFFICIENCY, FLOW	map	curve	point
EFF-POLY	COEF1, COEF2, COEF3, COEF4	map	curve	—
STAGE-DATA	SUCT-NOZ-DIA, SUCT-K-FACT, ACT-SH-SPEED, REF-SH-SPEED, FANEXPH, FANEXPE, FANEXPP, SCL-FACTOR1, SCL-FACTOR2	stage	—	—
WHEEL-DATA	FANEXPH, FANEXPE, FANEXPP, IMPELLER-DIA, SCL-FACTOR1, SCL-FACTOR2	stage	wheel	—
SHAFT-SPEED	SHAFT-SPEED	map	curve	—
MACH-NO	MACH-NO	map	curve	—
HCURVE	NPOINTS, INCR, PDROPS	curveno	—	—

Block Results

Description	Sentence	Variable	ID1
Total brake horsepower	RESULTS	BRAKE-POWER	—
Net work	RESULTS	NET-WORK	—
Total cooling duty	RESULTS	QCALC	—
Net cooling duty	RESULTS	NET-DUTY	—
Brake horsepower	PROFILE	BRAKE-POWER†	stage
Cooling duty	PROFILE	QCALC†	stage
Pressure (compression outlet)	PROFILE	COMPR-PRES†	stage
Temperature (compression outlet)	PROFILE	COMPR-TEMP†	stage
Pressure (cooling outlet)	PROFILE	COOLER-PRES†	stage
Temperature (cooling outlet)	PROFILE	COOLER-TEMP†	stage
Cooler vapor fraction	PROFILE	COOLER-VFRAC†	stage

Stage-by-stage performance results:

Description	Sentence	Variable	ID1	ID2
Percent above surge	STAGE-RESULTS	ABOVE-SURGE	stage	—
Percent below stonewall	STAGE-RESULTS	BELOW-SWALL	stage	—
Calculated compressor shaft speed	STAGE-RESULTS	SHAFT-SPEED	stage	—
Specific shaft speed	STAGE-RESULTS	SP-SPEED	stage	—
Sonic velocity of gas at suction	STAGE-RESULTS	SUCT-SONIC-V	stage	—

Wheel-by-wheel performance results:

Description	Sentence	Variable	ID1	ID2
Percent above surge	WHEEL-RESULTS	ABOVE-SURGE	stage	wheel
Percent below stonewall	WHEEL-RESULTS	BELOW-SWALL	stage	wheel
Calculated compressor shaft speed	WHEEL-RESULTS	SHAFT-SPEED	stage	wheel
Specific shaft speed	WHEEL-RESULTS	SP-SPEED	stage	wheel
Sonic velocity of gas at suction	WHEEL-RESULTS	SUCT-SONIC-V	stage	wheel
Specific diameter	WHEEL-RESULTS	SP-DIAM	stage	wheel
Head coefficient	WHEEL-RESULTS	HEAD-COEF	stage	wheel
Flow coefficient	WHEEL-RESULTS	FLOW-COEF	stage	wheel
Inlet Mach number	WHEEL-RESULTS	IN-MACH-NO	stage	wheel
Rotor tip Mach number	WHEEL-RESULTS	RT-MACH-NO	stage	wheel

† You can also access variables using the VECTOR-DEF sentence. See Chapter 29.

Notes

1 The polytropic efficiency η_p is used in the equation for the polytropic compression ratio:

$$\frac{n-1}{n} = \left(\frac{k-1}{k}\right) / \eta_p$$

The basic compressor relation is:

$$\Delta h = \frac{P_{in} V_{in}}{\eta_p \left(\frac{n-1}{n}\right)} \left[\left(\frac{P_{out}}{P_{in}}\right)^{\left(\frac{n-1}{n}\right)} - 1 \right]$$

Where:

n	=	Polytropic coefficient
k	=	Heat capacity ratio C_p/C_v
η_p	=	Polytropic efficiency
Δh	=	Enthalpy change per mole
P	=	Pressure
V	=	Volume

2 The isentropic efficiency η_s for compression is:

$$\eta_s = \frac{h_{out}^s - h_{in}}{h_{out} - h_{in}}$$

The isentropic efficiency η_s for expansion is:

$$\eta_s = \frac{h_{out} - h_{in}}{h_{out}^s - h_{in}}$$

Where:

h	=	Molar enthalpy
h_{out}^s	=	Outlet molar enthalpy, assuming isentropic compression/expansion to the specified outlet pressure

3 The mechanical efficiency η_m is:

$IHP = F\Delta h$
$BHP = IHP / \eta_m$ (for compression processes)
$BHP = IHP \times \eta_m$ (for expansion processes)

Power loss, PLOSS, can be used to calculate the brake horsepower, in place of the mechanical efficiency:

$BHP = IHP + PLOSS$ (for compression processes)
$BHP = IHP - PLOSS$ (for expansion processes)

Where:

IHP = Indicated horsepower

F = Mole flow rate

Δh = Enthalpy change per mole

BHP = Brake horsepower

η_m = Mechanical efficiency

$PLOSS$ = Power loss

4 Parasitic pressure loss at the suction nozzle of a compression stage is given by the equation:

$$Pdrop = K * \rho * (V^2) / (2*g)$$

Where:

K = Velocity head multiplier

ρ = Density

V = Linear velocity of process gas at suction conditions

g = Gravitational constant

5 When head or head coefficient curves are specified, the data can be based on either actual head or thermodynamic head. Actual and thermodynamic heads are related by the following equations:

Hact = Hpoly / Peff for polytropic path
Hact = Hisen / Ieff for isentropic path (for compression processes)
Hact = Hisen $\times$ *Ieff* for isentropic path (for expansion processes)

Where:

Hact = Actual head

Hpoly = Polytropic head

Peff = Polytropic efficiency

Hisen = Isentropic head

Ieff = Isentropic efficiency

6 You can specify either tables or polynomials for all curves entered. You may not mix tables and polynomials. You can enter only one of the following for a given compressor stage: HEAD-TABLE, HEAD-POLY, HEADC-TABLE, HEADC-POLY, POWER-TABLE, POWER-POLY, PRES-TABLE, PRES-POLY, PRATIO-TABLE, PRATIO-POLY, DELP-TABLE, DELP-POLY, HEAD-CORR.

7 When you specify performance curves as tables, you must give at least four data points in each table. Aspen Plus fits parameters for each table using a cubic spline.

8 The head coefficient is defined by the following equation:

$H_c = H * g / (\pi * Shspd * ImpDiam)^2$

Where:

H_C	=	Head coefficient
H	=	Head developed
g	=	Gravitational constant
Shspd	=	Shaft speed
ImpDiam	=	Impeller diameter of compressor wheel

The flow coefficient is defined by the following equation:

$F_c = Vfl_{in} / (Shspd * ImpDiam^3)$

Where:

F_C	=	Flow coefficient
Vfl_{in}	=	Volumetric flow rate at suction conditions
Shspd	=	Shaft speed
ImpDiam	=	Impeller diameter of compressor wheel

9 You can specify efficiency either as a scalar (in the PARAM sentence) or a curve (in either the EFF-TABLE or the EFF-POLY sentences, or EFF-CORR if the HEAD-CORR sentence is specified).

10 When multiple performance curves at multiple shaft speeds are supplied, Aspen Plus uses linear interpolation between the speeds to analyze performance.

11 When multiple performance curves at multiple Mach numbers are supplied, Aspen Plus uses linear interpolation between the Mach numbers to analyze performance.

12 The head developed for a compressor to change the pressure of a stream from the inlet pressure P_1 to the outlet pressure P_2 is given by:

$$HEAD = \int_{p1}^{p2} VdP$$

where *V* is the molar volume and subscripts 1 and 2 refer to inlet and outlet conditions, respectively. Two integration methods are provided for the polytropic and positive displacement model calculations using piecewise integration:

Direct method

Applying the gas law *PV* = *ZRT* and using the average point for each interval, given the number of intervals between P_1 and P_2, subpath *i* for head developed can be written as:

$$HEAD^i = R(ZT)_{av} \ln\left(\frac{P_2^i}{P_1^i}\right)$$

The total polytropic head is the sum of the subpath heads:

$$HEAD = \sum_i HEAD^i$$

n-Method

In a polytropic compression process, the relation of pressure *P* to volume *V* is expressed by the following equation:

$PV^n = C = Constant$

where n is the polytropic exponent. The n-method is to integrate head equation, between P_1 and P_2, over a small interval such that a constant n is assumed. For subpath *i*, the head developed can be written as:

$$HEAD^i = \frac{P_1^i V_1^i}{\left(\frac{n-1}{n}\right)}\left[\left(\frac{P_2^i}{P_1^i}\right)^{\frac{n-1}{n}} - 1\right]$$

21 Pipes and Valves

This chapter describes the input language for the pipeline, pipe, and valve models. The models are:

Model	Description	Purpose	Use
PIPELINE	Pipeline calculation	Calculate pressure drop in a straight pipe or annular space	Successive PIPELINE blocks simulate a piping network that includes wellbores and flowlines
PIPE	Single-segment pipe calculation	Calculate pressure drop in a single-segment pipe	PIPE simulates a single-segment pipe including fittings and valves
VALVE	Valve calculation	Calculate pressure drop or flow coefficient for a valve	VALVE simulates a control valve or pressure changer

PIPELINE: Pipeline Calculation

Input Language for PIPELINE

BLOCK **blockid** **PIPELINE**
PARAM *keyword=value*

Optional keywords:

PRES-CALC FLOW-CALC THERMAL INTEGRATION CL-FORM-METH FRIC-DOWNHILL FRIC-HORIZ FRIC-INCL FRIC-VERTICA HOLDUP-DOWNH HOLDUP-HORIZ HOLDUP-INCL HOLDUP-VERTI RECY-REUSE EDIT-REUSE NPHASE PHASE INT-METHOD INT-TOL CORR-METHOD CORR-TOL-RATIO TOL MAXIT

Optional keywords less frequently used:

P-RECOV SLIP MINVOL DOWNHILL-MAX DOWNHILL-MIN HINIT REYN-TRAN INTERR ORKDEN-KEY NIKLIN ORKWLR BB1 BB2 BB3 BB4 BB5 BB6 BB7 BB8 BB9 BB10

NODE **nodeno** **name** *keyword=value*

Keywords:

X Y ELEV P T TAMB

Optional keyword:

CERO

SEGMENT **segno** *keyword=value* **/ ...**

Keywords:

INNODE OUTNODE ID UVAL LENGTH ANGLE

Optional keywords:

OD ROUGH HEATFLUX EFFICIENCY

TABLE-DEF *keyword=value*

Keywords:

P-T-TABLE PRES TEMP NPRES PMIN PMAX NTEMP TMIN TMAX

Optional keywords:

BLOCKID CBAR

PRINT *keyword=value*

Keywords:

TABLES BBFRIC BBHOLDUP GLPRINT REPRNT

SUBROUTINE *keyword=value*

Keywords:

HOLDUP PRES-DROP

USER-VECS *keyword=value*

Keywords:

NINTH NREALH NINTP NREALP NIWORKH NRWORKH NIWORKP NRWORKP

INTH value-list
REALH value-list
INTP value-list
REALP value-list

Input Language Description for PIPELINE

PARAM

Use to specify pipeline simulation options, integration parameters, frictional correlation options, Beggs and Brill correlation coefficients, and optional convergence parameters.

PRES-CALC..... Pressure calculation option. Use to specify whether inlet or outlet conditions are calculated.

PRES-CALC=OUTLET	Calculates outlet pipeline conditions given inlet conditions (Default)
PRES-CALC=INLET	Calculates inlet pipeline conditions given outlet conditions

FLOW-CALC..... Flow calculation option. Use to specify whether inlet or outlet stream composition and flow are calculated.

FLOW-CALC=OUTLET	Calculates outlet stream composition and flow from the inlet stream (Default)
FLOW-CALC=INLET	Calculates inlet stream composition and flow from the outlet stream

THERMAL ..... Thermal simulation option. Use to control heat-transfer calculations.

THERMAL=YES	Calculates temperatures using energy balance
THERMAL=NO	Assumes linear temperature profile between node temperature(s) entered by user (Default)

INTEGRATION..... Numerical integration option:

INTEGRATION=YES	Uses numerical integration (Default)
INTEGRATION=NO	Uses one of the closed-form methods

CL-FORM-METH..... One-phase method for closed-form calculation. Use when INTEGRATION=NO.

CL-FORM-METH=AGA	AGA (Default)
CL-FORM-METH= HAZEN-WILL	Hazen-Williams
CL-FORM-METH= OLIPHANT	Oliphant
CL-FORM-METH= PANHANDLE-A	Panhandle A
CL-FORM-METH= PANHANDLE-B	Panhandle B
CL-FORM-METH=SMITH	Smith
CL-FORM-METH= WEYMOUTH	Weymouth

FRIC-DOWNHILL..... Two-phase frictional pressure-drop correlation option for downhill flow. Use when inclination angles are less than -2 degrees from horizontal.

	FRIC-DOWNHILL=BEGGS-BRILL	Beggs and Brill (Default)
	FRIC-DOWNHILL=DARCY	Darcy. Assumes no slip.
	FRIC-DOWNHILL=SLACK	Slack
	FRIC-DOWNHILL=USER-SUBS	User-supplied subroutine
FRIC-HORIZ	Two-phase frictional pressure-drop correlation option for horizontal flow. Use when the inclination angles range between -2 and +2 degrees from horizontal.	
	FRIC-HORIZ=BEGGS-BRILL	Beggs and Brill (Default)
	FRIC-HORIZ=DARCY	Darcy. Assumes no slip.
	FRIC-HORIZ=DUKLER	Dukler
	FRIC-HORIZ=LOCK-MART	Lockhart-Martinelli
	FRIC-HORIZ=USER-SUBS	User-supplied subroutine
FRIC-INCL	Two-phase frictional pressure-drop correlation option for inclined flow. Use when the inclination angles range between +2 and +45 degrees from horizontal.	
	FRIC-INCL=AWR	Angel-Welchon-Ros
	FRIC-INCL=BEGGS-BRILL	Beggs and Brill (Default)
	FRIC-INCL=DARCY	Darcy. Assumes no slip.
	FRIC-INCL=DUKLER	Dukler
	FRIC-INCL=H-BROWN	Hagedorn-Brown
	FRIC-INCL=ORKI	Orkiszewski
	FRIC-INCL=USER-SUBS	User-supplied subroutine
FRIC-VERTICA	Two-phase frictional pressure-drop correlation option for vertical flow. Use when inclination angles are greater than +45 degrees from horizontal.	
	FRIC-VERTICA=AWR	Angel-Welchon-Ros
	FRIC-VERTICA=BEGGS-BRILL	Beggs and Brill (Default)
	FRIC-VERTICA=DARCY	Darcy. Assumes no slip.
	FRIC-VERTICA=H-BROWN	Hagedorn-Brown
	FRIC-VERTICA=ORKI	Orkiszewski
	FRIC-VERTICA=USER-SUBS	User-supplied subroutine
HOLDUP-DOWNH	Two-phase liquid holdup correlation option for downhill flow. Use when inclination angles are less than -2 degrees from horizontal.	
	HOLDUP-DOWNH=BEGGS-BRILL	Beggs and Brill (Default)
	HOLDUP-DOWNH=SLACK	Slack
	HOLDUP-DOWNH=USER-SUBS	User-supplied subroutine
HOLDUP-HORIZ	Two-phase liquid holdup correlation option for horizontal flow. Use when inclination angles range between -2 and +2 degrees from horizontal.	
	HOLDUP-HORIZ=BEGGS-BRILL	Beggs and Brill (Default)
	HOLDUP-HORIZ=EATON	Eaton
	HOLDUP-HORIZ=HOOG	Hoogendorn
	HOLDUP-HORIZ=HUGH	Hughmark

	HOLDUP-HORIZ=LOCK-MART	Lockhart-Martinelli
	HOLDUP-HORIZ=USER-SUBS	User-supplied subroutine
HOLDUP-INCL	Two-phase liquid holdup correlation option for inclined flow. Use when inclination angles range between +2 and +45 degrees from horizontal.	
	HOLDUP-INCL=AWR	Angel-Welchon-Ros
	HOLDUP-INCL=BEGGS-BRILL	Beggs and Brill (Default)
	HOLDUP-INCL=FLANIGAN	Flanigan
	HOLDUP-INCL=H-BROWN	Hagedorn-Brown
	HOLDUP-INCL=ORKI	Orkiszewski
	HOLDUP-INCL=USER-SUBS	User-supplied subroutine
HOLDUP-VERTI	Two-phase liquid holdup correlation option for vertical flow. Use when inclination angles are greater than +45 degrees from horizontal.	
	HOLDUP-VERTI=AWR	Angel-Welchon-Ros
	HOLDUP-VERTI=BEGGS-BRILL	Beggs and Brill (Default)
	HOLDUP-VERTI=H-BROWN	Hagedorn-Brown
	HOLDUP-VERTI=ORKI	Orkiszewski
	HOLDUP-VERTI=USER-SUBS	User-supplied subroutine
RECY-REUSE	Option to allow reuse of fluid property tables in convergence loops:	
	RECY-REUSE=YES	Reuses tables after initial iteration
	RECY-REUSE=NO	Recalculates tables for every iteration (Default)
EDIT-REUSE	Option to allow reuse of fluid property tables in edit runs:	
	EDIT-REUSE=YES	Reuses tables after initial execution
	EDIT-REUSE=NO	Recalculates tables for every execution (Default)
NPHASE	Number of phases for flash calculations. For gas systems in the dense-phase region, a value of NPHASE=1 is recommended.	
	NPHASE=1	One-phase calculation
	NPHASE=2	Two-phase flash (Default)
	NPHASE=3	Three-phase flash
PHASE	Specifies the phase when NPHASE=1:	
	PHASE=V	Vapor (Default)
	PHASE=L	Liquid
INT-METHOD	Integration method. Use when INTEGRATION=YES.	
	INT-METHOD=GEAR	Uses Gear's method (Default)
	INT-METHOD=HAMMING	Uses Hamming's predictor-corrector method
INT-TOL	Convergence tolerance for integration procedure. Use when INT-METHOD=GEAR. (Default=1×10^{-4})	
CORR-METHOD	Corrector convergence method. Use when INT-METHOD=GEAR.	
	CORR-METHOD=DIRECT	Direct substitution. Derivatives are not required
	CORR-METHOD=NEWTON	Newton method. Aspen Plus computes numerical derivatives whenever a new Jacobian is required. (Default)

CORR-TOL-RATIO..... Ratio of the corrector tolerance to the integration tolerance. Use when INT-METHOD=GEAR. (Default=0.1)

TOL ..... Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

MAXIT..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.)
(See Chapter 45.)

P-RECOV ..... Downhill pressure recovery option. Sets elevational pressure change to zero for downhill flow. See FRIC-DOWNHILL for definition of downhill.

P-RECOV=YES	Sets elevational pressure change to zero
P-RECOV=NO	Calculates elevational pressure change (Default)

SLIP..... Option to set liquid holdup equal to the flowing volume fraction in two-phase flow. This implies that the vapor and liquid travel at equal velocity, with no slip relative to each other.

SLIP=YES	Calculates holdup, as specified in HOLDUP keywords (Default)
SLIP=NO	Sets holdup equal to flowing volume fraction

MINVOL ..... Minimum phase volume fraction. This fraction is measured at flowing conditions, which a phase must occupy, for two-phase flow to occur. (Default=$1x10^{-4}$)

DOWNHILL-MAX ..... Largest elevation angle for which the P-RECOV option will set the elevation pressure change to zero. Aspen Plus measures the angle in degrees from horizontal. (Default=-2)

DOWNHILL-MIN..... Smallest elevation angle for which the P-RECOV option will set the elevation pressure change to zero. Aspen Plus measures the angle in degrees from horizontal. (Default=-45)

HINIT ..... Initial integration step-size, expressed as a fraction of the segment length (0<HINIT<1) (Default=0.01)

REYN-TRAN..... Reynolds number for laminar-to-turbulent flow transition (Default=3000)

INTERR ..... Allowable integration error. If the estimated error in the pressure calculated by the integration routine exceeds this value, the integration step-size is halved. If the error is less than two percent of INTERR, the step-size is doubled. Use when INT-METHOD=HAMMING. (Default=1 psi)

ORKDEN-KEY ..... Orkiszewski modified gas density key. The modified gas density for frictional pressure-drop in the mist flow regime is used for calculating the elevational pressure-drop in the Orkiszewski method.

ORKDEN-KEY=YES	Uses modified gas density
ORKDEN-KEY=NO	Uses actual gas density (Default)

NIKLIN ..... Niklin bubble-rise velocity key. The Niklin method is used for calculating bubble-rise velocity in the Orkiszewski routine.

NIKLIN=YES	Uses Niklin modification
NIKLIN=NO	Uses original Orkiszewski method (Default)

ORKWLR ..... Water/liquid ratio at which the Orkiszewski correlation considers water to be the continuous liquid phase. (Default=0.75)

BB1 through BB9 ..... User-supplied coefficients for the Beggs & Brill liquid holdup correlation. See Table 22.1 on page 22-12 for defaults.

BB10..... Beggs & Brill two-phase friction factor multiplier. The multiplier adjusts the computed friction factor. It can be used to match field data. (Default=1.00)

NODE

Use to enter node information for the pipeline. You must enter at least two nodes to define a single PIPELINE block. You do not have to list the nodes in the order that defines pipe inlet to outlet, because PIPELINE sorts this data. (Any value entered for T or TAMB will be passed on to subsequent nodes, if these keywords are omitted on the following nodes.) If you do not specify LENGTH and ANGLE for the corresponding SEGMENT, you must specify X, Y, and ELEV for each NODE sentence.

nodeno..... Positive integer number ranging from 1 to the total number of nodes

name ..... A unique, four-character alphanumeric name that must be entered to identify each pipeline node

X..... X-position of the user-defined Cartesian coordinate system (Default=0)

Y..... Y-position of the user-defined Cartesian coordinate system (Default=0)

ELEV ..... Elevation of the user-defined Cartesian coordinate system (Default=0)

P..... Node pressure. This value can only be entered for the inlet or outlet node of the pipeline, depending on the direction of calculation.

T..... Node temperature. When THERMAL=NO, you can enter node temperatures to establish a flowing fluid profile.

TAMB ..... Ambient temperature. When THERMAL=YES, you must enter values for the ambient temperature.

CERO..... Erosional velocity calculation constant (Default=100)

SEGMENT

Use to enter segment information for the pipeline. You must enter at least one segment to define a single PIPELINE block. The total number of segments must be one less than the number of nodes. You do not have to list the segments in the order that defines pipe inlet to outlet, because PIPELINE sorts this data. Any value entered for ID, UVAL, ROUGH, HEATFLUX, or EFFICIENCY will be passed on to subsequent segments, if these keywords are omitted on the following segments. If you do not specify X, Y, and ELEV for the corresponding NODE, you must specify LENGTH and ANGLE for each SEGMENT sentence.

segno..... Positive integer number ranging from 1 to the total number of segments

INNODE ..... Inlet node name of segment

OUTNODE..... Outlet node name of segment

ID ..... Inner diameter of the pipe segment for tubular flow, or outer diameter of the inner pipe for annular flow

UVAL..... Overall heat transfer coefficient. Required only when THERMAL=YES. (Default 0)

LENGTH..... Segment length. If you do not specify nodal position coordinates (X, Y, ELEV), you must enter the segment length here.

ANGLE Segment angle. If you do not specify nodal position coordinates (X, Y, ELEV), you must enter the segment angle here. The angle is measured from the horizontal.

OD The inner diameter of the outer pipe for annular flow. Use a positive entry to determine whether to perform an annular flow calculation.

ROUGH Pipe roughness (Default=0.0018 in.)

HEATFLUX Uniform heat added to segment. Use only when THERMAL=YES (Default=0). The units for HEATFLUX are BTU/hr-ft for the English engineering system (ENG) and Watt/m for the International system (SI).

EFFICIENCY Pipe efficiency factor. The calculated frictional component of the pressure gradient is divided by this factor (Default=1.0). Also used as the pipe C-factor when CL-FORM-METH=HAZEN-WILL.

TABLE-DEF

Use to specify the pressure and temperature grid for which fluid properties are calculated, or to specify that the properties are to be calculated exactly at each integration step. The grid can contain a maximum of 15 pressures and 10 temperatures. Pressure and temperature grid can be specified by using lists (PRES and TEMP), or by specifying the number of points and the maximum and minimum values. The property grids from a previously executed PIPELINE block can be accessed in the same flowsheet simulation by using the keyword BLOCKID.

P-T-TABLE Specifies whether to use a pressure-temperature grid, or to calculate fluid properties rigorously.

P-T-TABLE=NO	Does not create a pressure-temperature grid. Calculates the properties rigorously at each integration step. (Default)
P-T-TABLE=YES	Creates a pressure-temperature grid

PRES List of pressures for the pressure-temperature grid

TEMP List of temperatures for the pressure-temperature grid

NPRES Number of pressures in the grid (maximum of 15)

PMIN Lowest pressure in the grid

PMAX Highest pressure in the grid

NTEMP Number of temperatures in the grid (maximum of 10)

TMIN Lowest temperature in the grid

TMAX Highest temperature in the grid

BLOCKID Block ID of a previously executed PIPELINE block, from which the property grid is to be recovered

CBAR Cricondenbar. Use when part of the pressure-temperature grid lies in the dense-phase region. Specifying the phase envelope cricondenbar helps smooth out problems that occur when interpolating property values that cross the all-vapor/all-liquid transition line. The all-vapor/all-liquid transition line is typically predicted by equation-of-state methods in the dense-phase region.

PRINT

Use to set the output options.

TABLES Fluid property table output option:

TABLES=NO	Does not print tables (Default)
TABLES=PROP	Prints tables showing each property over the P/T grid

		TABLES=PT	Prints tables showing all properties at each P/T grid point
	BBFRIC	Beggs and Brill two-phase friction factor print option:	
		BBFRIC=NO	Does not print (Default)
		BBFRIC=YES	Prints diagnostics for each friction factor calculation
	BBHOLDUP	Beggs and Brill liquid holdup print option:	
		BBHOLDUP=NO	Does not print (Default)
		BBHOLDUP=YES	Prints diagnostics for each holdup calculation
	GLPRINT	Flow rate units option:	
		GLPRINT=MASS	Prints fluid flow rates at each node in MASS-FLOW units. (Default)
	REPRNT	Reynolds number print option. This option controls diagnostics from the Colebrook friction factor calculation.	
		REPRNT=0	No printout
		REPRNT=1	Prints each time the Reynolds number changes by 5%
		REPRNT=2	Prints each time the friction factor is calculated
SUBROUTINE	Use to specify user-supplied subroutine names for holdup and/or pressure-drop calculations. For details on writing these user-supplied subroutines, see *Aspen Plus User Models*, Chapter 17.		
	HOLDUP	Name of a user-supplied FORTRAN subroutine to calculate liquid holdup in two-phase flow	
	PRES-DROP	Name of a user-supplied FORTRAN subroutine to calculate pressure-drop derivatives in two-phase flow	
USER-VECS	Use to define the lengths of arrays for user-supplied holdup and pressure-drop subroutines.		
	NINTH	Length of integer parameter array for the user-supplied holdup subroutine	
	NREALH	Length of real parameter array for the user-supplied holdup subroutine	
	NINTP	Length of integer parameter array for the user-supplied pressure-drop subroutine	
	NREALP	Length of real parameter array for the user-supplied pressure-drop subroutine	
	NIWORKH	Length of integer workspace array for the user-supplied holdup subroutine	
	NRWORKH	Length of real workspace array for the user-supplied holdup subroutine	
	NIWORKP	Length of integer workspace array for the user-supplied pressure-drop subroutine	
	NRWORKP	Length of real workspace array for the user-supplied pressure-drop subroutine	
INTH	Use to enter values for the integer parameter array of the user-supplied holdup subroutine.		
	value-list	List of integer values	
REALH	Use to enter values for the real parameter array of the user-supplied holdup subroutine.		
	value-list	List of real values	

INTP Use to enter values for the integer parameter array of the user-supplied pressure-drop subroutine.

value-list ..... List of integer values

REALP Use to enter values for the real parameter array of the user-supplied pressure-drop subroutine.

value-list ..... List of real values

Table 22.1 Beggs and Brill Liquid Holdup Correlation Parameters

Flow Regime	Name	Description
Segregated	BB1	Leading coefficient, A (Default=0.98)
	BB2	Liquid volume fraction exponent, Alpha (Default=0.4846)
	BB3	Froude number exponent, Beta (Default=0.0868)
Intermittent	BB4	Leading coefficient, A (Default=0.845)
	BB5	Liquid volume fraction exponent, Alpha (Default=0.5351)
	BB6	Froude number exponent, Beta (Default=0.0173)
Distributed	BB7	Leading coefficient, A (Default=1.065)
	BB8	Liquid volume fraction exponent, Alpha (Default=0.5824)
	BB9	Froude number exponent, Beta (Default=0.0609)

Accessing Variables in PIPELINE

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	Element
PARAM	MAXIT, TOL, MINVOL, DOWNHILL-MAX, DOWNHILL-MIN, HINIT, REYN-TRAN, INTERR, ORKWLR, BB1, BB2, BB3, BB4, BB5, BB6, BB7, BB8, BB9, BB10	—	—
NODE	X, Y, ELEV, P, T, TAMB, CERO	nodeno	—
SEGMENT	ID, UVAL, LENGTH, ANGLE, OD, ROUGH, HEATFLUX, EFFICIENCY	segno	—
TABLE-DEF	PRES, TEMP, NPRES, PMIN, PMAX, NTEMP, TMIN, TMAX, CBAR	—	†

† Position of a value entered for PRES and TEMP in the TABLE-DEF sentence. For other variables, leave element blank.

Block Results

Description	Sentence	Variable	ID1
Node pressure	NODE	PCALC	nodeno
Node temperature	NODE	TCALC	nodeno
Node mixture velocity	NODE	VMIX	nodeno
Node erosional velocity	NODE	VERO	nodeno
Node flow regime	NODE	REGIME	nodeno
Segment friction pressure loss	SEGMENT	DPFRIC	segno
Segment elevation pressure loss	SEGMENT	DPELEV	segno
Segment acceleration pressure loss	SEGMENT	DPACC	segno
Segment total pressure loss	SEGMENT	DPTOTL	segno
Segment liquid holdup fraction	SEGMENT	HL-FRAC	segno
Segment calculated length	SEGMENT	LENGTH-CALC	segno
Segment calculated angle	SEGMENT	ANGLE-CALC	segno
Total liquid holdup	RESULTS	HLTOTAL	—
Inlet stream heat difference	RESULTS	QDIFF	—
Stream total mass flow rate	RESULTS	MASSRATE	—
Calculated pressure drop	RESULTS	DPPIDE	—

PIPE: Single-Segment Pipe Calculation

Input Language for PIPE

BLOCK **blockid** **PIPE**
PARAM *keyword=value*

Keywords:

LENGTH **IN-DIAM**

Optional keywords:

ELEVATION **ANGLE** **MATERIAL** **SCHEDULE** **NOM-DIAM** **ROUGHNESS** **PRES-CALC** **FLOW-CALC** **T-OUT** **P-OUT** **C-EROSION** **NPHASE** **PHASE** **MAXIT** **TOL** **NPOINT** **CALCDIA**

METHODS

Keywords:

TYPE **T-IN** **TAMB-IN** **TAMB-OUT** **H-T-COEFF** **FLUX** **P-T-TABLE** **EFFICIENCY** **METHOD** **CL-FORM-METH** **PROP-SETS** **FRIC-DOWNHIL** **FRIC-HORIZ** **FRIC-INCL** **FRIC-VERTICA** **HOLDUP-DOWNH** **HOLDUP-HORIZ** **HOLDUP-INCL** **HOLDUP-VERTI** **H-W-COEFF**

TABLE-DEF *keyword=value*

Keywords:

TEMP **PRES** **TMIN** **TMAX** **NTEMP** **PMIN** **PMAX** **NPRES** **RECY-REUSE** **EDIT-REUSE** **BLOCKID** **CBAR** **TABLES**

SUBROUTINE *keyword=value*

Keywords:

HOLDUP PRES-DROP DIAMETER

USER-VECS *keyword=value*

Keywords:

NINTH NREALH NINTP NREALP NINTD NREALD NIWORKH NRWORKH
NIWORKP NRWORKP NIWORKD NRWORKD

INTH value-list
REALH value-list
INTP value-list
REALP value-list
INTD value-list
REALD value-list
CONVERGENCE *keyword=value*

Keywords:

HINIT CORR-METHOD CORR-TOL-RAT INT-TOL BB1 BB2 BB3 BB4 BB5 BB6 BB7 BB8 BB9 BB10 CDPDL-TOL

FITTINGS *keyword=value*

Keywords:

CONNECTIONS ELBOWS STRAIGHT-TEE BRANCHED-TEE GATE-VALVES BUTTERFLY-VA MISC-L-D MISC-L-D-LAB MISC-K K-LABEL PIPE-ENTRANC ENTRANCE-RD PIPE-EXIT ENLARGEMENT E-ANGLE E-DIAM CONTRACTION C-ANGLE C-DIAM ORIFICE ORIFICE-DIAM ORIFICE-THIC

Input Language Description for PIPE

PARAM

Use to specify pipe dimensions, calculation options, and flash parameters. You must enter LENGTH and DIAM.

LENGTH..... Pipe length

IN-DIAM ..... Pipe diameter

ELEVATION ..... Change in elevation from pipe entrance to exit. Enter a positive value for uphill flow and a negative value for downhill flow. You cannot enter ELEVATION if you specify ANGLE. (Default=0)

ANGLE..... Pipe angle measured from the horizontal, where SIN (ANGLE)=ELEVATION/LENGTH. You cannot enter ANGLE if you specify ELEVATION. (Default=0)

MATERIAL..... Pipe material of construction. This value may be generated by the user interface. It is never required for calculations.

SCHEDULE..... Pipe schedule. This value may be generated by the user interface. It is never required for calculations.

NOM-DIAM..... Pipe nominal diameter. This value may be generated by the user interface. It is never required for calculations.

ROUGHNESS..... Pipe absolute roughness (Default=$1.5x10^{-4}$ ft.)

PRES-CALC..... Pressure calculation option. Use to specify whether inlet or outlet conditions are calculated.

PRES-CALC=OUTLET	Calculates outlet pipe conditions given inlet conditions (Default)
PRES-CALC=INLET	Calculates inlet pipe conditions given outlet conditions

FLOW-CALC..... Flow calculation option. Use to specify whether inlet or outlet stream composition and flow are calculated.

FLOW-CALC=OUTLET	Calculates outlet stream composition and flow from inlet conditions (Default)
FLOW-CALC=INLET	Calculates inlet stream composition and flow from outlet conditions

T-OUT ..... Optional outlet temperature when PRES-CALC=INLET, or when TYPE=T-SPEC and PRES-CALC=OUTLET

P-OUT ..... Optional outlet pressure when PRES-CALC=INLET

C-EROSION ..... Coefficient of erosion

NPHASE ..... Number of phases for flash calculations. For gas systems in the dense-phase region, a value of NPHASE=1 is recommended.

NPHASE=1	One-phase calculation
NPHASE=2	Two-phase flash (Default)
NPHASE=3	Three-phase flash

PHASE..... Specifies the phase when NPHASE=1:

PHASE=V	Vapor (Default)
PHASE=L	Liquid

MAXIT..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

TOL ..... Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

NPOINT..... Number of equally-spaced points along the pipe. Aspen Plus uses the points for the profile printed in the block report. This profile is only generated when METHOD=INTEGRATE. (Default=10)

CALCDIA .....

CALCDIA=1	Compute Pipe inner diameter using user subroutine
CALCDIA=0	Do not use user subroutine to compute Pipe inner diameter (Default)

METHODS

Use to specify type of calculation, temperature and pressure values, and frictional and holdup correlations. You must specify TYPE.

TYPE ..... Type of calculations (No default):

TYPE=T-SPEC	Constant temperature or temperature profile
TYPE=THERMAL	Thermal calculations using constant flux or heat transfer with surroundings
TYPE=ADIABATIC	Constant enthalpy calculations

T-IN ..... Optional inlet temperature when TYPE=T-SPEC and PRES-CALC=INLET

TAMB-IN ..... Ambient temperature at the pipe entrance, used when TYPE=THERMAL. You must enter TAMB-IN if FLUX is not entered. (No default)

TAMB-OUT ..... Ambient temperature at the pipe exit, used when TYPE=THERMAL. You must enter TAMB-OUT if FLUX is not entered. (No default)

H-T-COEFF ..... Heat transfer coefficient. You must enter H-T-COEFF if FLUX is not entered and TYPE=THERMAL. (No default)

FLUX ..... Heat flux. You must enter FLUX when TAMB-IN and H-T-COEFF are not entered and TYPE=THERMAL. The units for FLUX are BTU/hr-ft for the English engineering system (ENG) and Watt/m for the International system (SI). (No default)

P-T-TABLE..... Specifies whether to use a pressure-temperature grid, or to calculate fluid properties rigorously.

P-T-TABLE=NO	Does not create a pressure-temperature grid. Calculates the properties rigorously at each integration step. (Default)
P-T-TABLE=YES	Creates a pressure-temperature grid

EFFICIENCY ..... Pipe efficiency factor. The calculated frictional component of the pressure gradient is divided by this factor. (Default=1.0)

METHOD..... Specifies the solution method:

METHOD=INTEGRATE	Uses numerical integration (Default)
METHOD=CLOSED-FORM	Uses one of the closed form methods
METHOD=CONST-DP-DL	Calculates the derivative dP/dL at the pipe entrance and exit, and uses the average in pipe pressure-drop calculations

CL-FORM-METH..... Closed form method when METHOD=CLOSED-FORM

CL-FORM-METH=AGA	AGA (Default)
CL-FORM-METH= HAZEN-WILL	Hazen-Williams
CL-FORM-METH= OLIPHANT	Oliphant
CL-FORM-METH= PANHANDLE-A	Panhandle A
CL-FORM-METH= PANHANDLE-B	Panhandle B
CL-FORM-METH=SMITH	Smith
CL-FORM-METH= WEYMOUTH	Weymouth

PROP-SETS ..... List of property set IDs. The properties will be calculated at profile points. (See NPOINT in the PARAM sentence.) PROP-SETS is allowed only when METHOD=INTEGRATE.

FRIC-DOWNHIL ..... Two-phase frictional pressure-drop correlation option for downhill flow. Use when inclination angles are less than -2 degrees from horizontal. You must enter a value when METHOD=INTEGRATE or CONST-DP-DL.

FRIC-DOWNHIL= BEGGS-BRILL	Beggs and Brill (Default)
FRIC-DOWNHIL=DARCY	Darcy. Assumes no slip.
FRIC-DOWNHIL=SLACK	Slack
FRIC-DOWNHIL= USER-SUBR	User-supplied subroutine

FRIC-HORIZ..... Two-phase frictional pressure-drop correlation option for horizontal flow. Use when inclination angles range between -2 and +2 degrees from horizontal. You must enter a value when METHOD=INTEGRATE or CONST-DP-DL:

FRIC-HORIZ= BEGGS-BRILL	Beggs and Brill (Default)
FRIC-HORIZ=DARCY	Darcy. Assumes no slip.
FRIC-HORIZ=DUKLER	Dukler
FRIC-HORIZ=LOCK-MART	Lockhart-Martinelli
FRIC-HORIZ=USER-SUBR	User-supplied subroutine

FRIC-INCL..... Two-phase frictional pressure-drop correlation option for inclined flow. Use when inclination angles range between +2 and +45 degrees from horizontal. You must enter a value when METHOD=INTEGRATE or CONST-DP-DL:

FRIC-INCL=AWR	Angel-Welchon-Ros
FRIC-INCL=BEGGS-BRILL	Beggs and Brill (Default)
FRIC-INCL=DARCY	Darcy. Assumes no slip.
FRIC-INCL=DUKLER	Dukler
FRIC-INCL=H-BROWN	Hagedorn-Brown
FRIC-INCL=ORKI	Orkiszewski
FRIC-INCL=USER-SUBR	User-supplied subroutine

FRIC-VERTICA ..... Two-phase frictional pressure-drop correlation option for vertical flow. Use when inclination angles are greater than +45 degrees from horizontal. You must enter a value when METHOD=INTEGRATE or CONST-DP-DL:

FRIC-VERTICA=AWR	Angel-Welchon-Ros
FRIC-VERTICA= BEGGS-BRILL	Beggs and Brill (Default)
FRIC-VERTICA=DARCY	Darcy. Assumes no slip.
FRIC-VERTICA=H-BROWN	Hagedorn-Brown
FRIC-VERTICA=ORKI	Orkiszewski
FRIC-VERTICA= USER-SUBR	User-supplied subroutine

HOLDUP-DOWNH ..... Two-phase liquid holdup correlation option for downhill flow. Use when inclination angles are less than -2 degrees from horizontal. You must enter a value when METHOD=INTEGRATE or CONST-DP-DL:.....

HOLDUP-DOWNH= BEGGS-BRILL	Beggs and Brill (Default)
HOLDUP-DOWNH=SLACK	Slack
HOLDUP-DOWNH= USER-SUBR	User-supplied subroutine

HOLDUP-HORIZ ..... Two-phase liquid holdup correlation option for horizontal flow. Use when inclination angles range between -2 and +2 degrees from horizontal. You must enter a value when METHOD=INTEGRATE or CONST-DP-DL:

HOLDUP-HORIZ= BEGGS-BRILL	Beggs and Brill (Default)
HOLDUP-HORIZ=EATON	Eaton
HOLDUP-HORIZ=HOOG	Hoogendorn
HOLDUP-HORIZ=HUGH	Hughmark
HOLDUP-HORIZ= LOCK-MART	Lockhart-Martinelli
HOLDUP-HORIZ= USER-SUBR	User-supplied subroutine

HOLDUP-INCL ..... Two-phase liquid holdup correlation option for inclined flow. Use when inclination angles range between +2 and +45 degrees from horizontal. You must enter a value when METHOD=INTEGRATE or CONST-DP-DL:

HOLDUP-INCL=AWR	Angel-Welchon-Ros
HOLDUP-INCL= BEGGS-BRILL	Beggs and Brill (Default)
HOLDUP-INCL=FLANIGAN	Flanigan
HOLDUP-INCL=H-BROWN	Hagedorn-Brown
HOLDUP-INCL=ORKI	Orkiszewski
HOLDUP-INCL= USER-SUBR	User-supplied subroutine

HOLDUP-VERTI ..... Two-phase liquid holdup correlation option for vertical flow. Use when inclination angles are greater than +45 degrees from horizontal. You must enter a value when METHOD=INTEGRATE or CONST-DP-DL:

HOLDUP-VERTI=AWR	Angel-Welchon-Ros
HOLDUP-VERTI= BEGGS-BRILL	Beggs and Brill (Default)
HOLDUP-VERTI= H-BROWN	Hagedorn-Brown
HOLDUP-VERTI=ORKI	Orkiszewski
HOLDUP-VERTI= USER-SUBR	User-supplied subroutine

H-W-COEFF ..... Hazen Williams coefficient. Used when CL-FORM-METH=HAZEN-WILL. (Default=100)

TABLE-DEF

Use to specify the pressure and temperature grid for which fluid properties are calculated, when P-T-TABLE=YES in the METHODS sentence. The grid can contain a maximum of 15 pressures and 10 temperatures. The pressure and temperature grid can be specified by using lists (PRES and TEMP), or by specifying the number of points and the maximum and minimum values. The property grids from a previously executed PIPE block can be accessed in the same flowsheet simulation by using the keyword BLOCKID.

TEMP..... List of temperatures for the pressure-temperature grid

PRES..... List of pressures for the pressure-temperature grid

TMIN..... Lowest temperature in the grid

TMAX ..... Highest temperature in the grid

NTEMP ..... Number of temperatures in the grid (maximum of 10)

PMIN..... Lowest pressure in the grid

PMAX ..... Highest pressure in the grid

NPRES..... Number of pressures in the grid (maximum of 15)

RECY-REUSE ..... Option to allow reuse of fluid property tables in convergence loops:

RECY-REUSE=YES	Reuses tables after initial iteration
RECY-REUSE=NO	Recalculates tables for every iteration (Default)

EDIT-REUSE..... Option to allow reuse of fluid property tables in edit runs:

EDIT-REUSE=YES	Reuses tables after initial execution
EDIT-REUSE=NO	Recalculates tables for every execution (Default)

BLOCKID..... Block ID of a previously executed PIPE block, from which the property grid is to be recovered

CBAR..... Cricondenbar. Use when part of the pressure-temperature grid lies in the dense-phase region. Specifying the phase envelope cricondenbar helps smooth out problems that occur when interpolating property values that cross the all-vapor/all-liquid transition line. The all-vapor/all-liquid transition line is typically predicted by equation-of-state methods in the dense-phase region.

TABLES ..... Fluid property table output option:

TABLES=NO	Does not print tables
TABLES=PROP	Prints tables showing each property over the P/T grid
TABLES=PT	Prints tables showing all properties at each P/T grid point

SUBROUTINE

Use to specify user-supplied subroutine names for holdup and/or pressure-drop calculations. For details on writing user-supplied subroutines, see *Aspen Plus User Models*, Chapter 17.

HOLDUP ..... Name of a user-supplied FORTRAN subroutine to calculate liquid holdup in two-phase flow

PRES-DROP..... Name of a user-supplied FORTRAN subroutine to calculate pressure-drop derivatives in two-phase flow

DIAMETER..... Name of a user-supplied FORTRAN subroutine to calculate Pipe inner diameter

USER-VECS

Use to define the lengths of arrays for user-supplied holdup and pressure-drop subroutines.

NINTH..... Length of integer parameter array for the user-supplied holdup subroutine

NREALH ..... Length of real parameter array for the user-supplied holdup subroutine

NINTP..... Length of integer parameter array for the user-supplied pressure-drop subroutine

NREALP..... Length of real parameter array for the user-supplied pressure-drop subroutine

NINTD..... Length of integer parameter array for the user-supplied diameter subroutine

NREALD ..... Length of real parameter array for the user-supplied diameter subroutine

NIWORKH ..... Length of integer workspace array for the user-supplied holdup subroutine

NRWORKH ..... Length of real workspace array for the user-supplied holdup subroutine

NIWORKP ..... Length of integer workspace array for the user-supplied pressure-drop subroutine

NRWORKP..... Length of real workspace array for the user-supplied pressure-drop subroutine

NIWORKD ..... Length of integer workspace array for the user-supplied diameter subroutine

NRWORKD ..... Length of real workspace array for the user-supplied diameter subroutine

INTH

Use to enter values for the integer parameter array of the user-supplied holdup subroutine.

value-list ..... List of integer values

REALH Use to enter values for the real parameter array of the user-supplied holdup subroutine.

value-list ..... List of real values

INTP Use to enter values for the integer parameter array of the user-supplied pressure-drop subroutine.

value-list ..... List of integer values

REALP Use to enter values for the real parameter array of the user-supplied pressure-drop subroutine.

value-list ..... List of real values

INTD Use to enter values for the integer parameter array of the user-supplied diameter subroutine.

value-list ..... List of integer values

REALD Use to enter values for the real parameter array of the user-supplied diameter subroutine.

value-list ..... List of real values

CONVERGENCE Use to specify optional convergence parameters and Beggs and Brill coefficients.

HINIT ..... Initial integration step-size, expressed as a fraction of the segment length (0<HINIT<1). Use when METHOD=INTEGRATE. (Default=0.01)

CORR-METHOD..... Corrector convergence method. Use when METHOD=INTEGRATE:

CORR-METHOD=DIRECT	Direct substitution. Derivatives are not required
CORR-METHOD=NEWTON	Newton method. Aspen Plus computes numerical derivatives whenever a new Jacobian is required. (Default)

CORR-TOL-RAT ..... Ratio of the corrector tolerance to the integration tolerance. Use when METHOD=INTEGRATE. (Default=0.1)

INT-TOL..... Convergence tolerance for integration procedure. Use when METHOD=INTEGRATE. (Default=$1x10^{-4}$)

BB1 through BB9 ..... User-supplied coefficients for the Beggs & Brill liquid holdup correlation. See Table 22.1 on page 22-12 for defaults.

BB10..... Beggs & Brill two-phase friction factor multiplier. The multiplier adjusts the computed friction factor. It can be used to match field data. (Default=1.00)

CDPDL-TOL ..... Tolerance used to determine whether a warning is generated when METHOD=CONST-DP-DL

FITTINGS Use to specify fittings, such as gate valves, elbows, and branched tees. The resistance due to fittings is converted to equivalent length and added to the pipe length to calculate total pressure drop.

CONNECTIONS..... Type of connection between pipe lengths:

CONNECTIONS= FLANGED-WELD	Flanged or welded connection (Default)
CONNECTIONS= SCREWED	Screwed connection

ELBOWS..... Number of 90º elbows in the pipe

STRAIGHT-TEE..... Number of straight tees in the pipe

BRANCHED-TEE..... Number of branched tees in the pipe

GATE-VALVES ..... Number of gate valves in the pipe

BUTTERFLY-VA..... Number of butterfly valves in the pipe

MISC-L-D ..... Miscellaneous L/D for other elements in the pipe

MISC-L-D-LAB..... A label describing the miscellaneous L/D (a string in double quotes)

MISC-K ..... Miscellaneous K factor for other elements in the pipe. K factor is defined as friction factor times the L/D associated with the element.

K-LABEL..... A label describing the miscellaneous K (a string in double quotes)

PIPE-ENTRANC ..... Type of fitting at the pipe entrance.

PIPE-ENTRANC = NONE	Do not account for pipe entrance fitting (default)
PIPE-ENTRANC = INWARD	Inward-projecting pipe entrance, K=0.78
PIPE-ENTRANC = FLUSH	Flush pipe entrance, K depends on R/D.

ENTRANCE-RD..... Entrance bend radius / pipe diameter. Use only with PIPE-ENTRANC = FLUSH.

ENTRANCE-RD = 0	Sharp-edged entrance
ENTRANCE-RD = "0.02"	R/D = 0.02
ENTRANCE-RD = "0.04"	R/D = 0.04
ENTRANCE-RD = "0.06"	R/D = 0.06
ENTRANCE-RD = "0.1"	R/D = 0.1
ENTRANCE-RD = ".15_AND_UP"	R/D = 0.15 or greater

PIPE-EXIT..... Whether to account for fitting at pipe exit

PIPE-EXIT = NO	Do not account for fitting at pipe exit. (Default)
PIPE-EXIT = YES	Add K=1.0 for pipe exit.

ENLARGEMENT..... Whether sudden enlargement fitting exists.

ENLARGEMENT = NO	No sudden enlargement. (Default)
ENLARGEMENT = YES	Sudden enlargement fitting exists.

E-ANGLE ..... Angle in sudden enlargement fitting.

E-DIAM ..... Diameter at other end of sudden enlargement fitting (not pipe diameter).

CONTRACTION..... Whether sudden contraction fitting exists.

CONTRACTION = NO	No sudden contraction. (Default)
CONTRACTION = YES	Sudden contraction fitting exists.

C-ANGLE ..... Angle in sudden contraction fitting.

C-DIAM ..... Diameter at other end of sudden contraction fitting (not pipe diameter).

ORIFICE..... Whether orifice plate exists.

ORIFICE = NO	No orifice plate. (Default)
ORIFICE = YES	Orifice plate exists.

ORIFICE-DIAM..... Diameter of orifice.

ORIFICE-THIC..... Thickness of orifice plate.

Accessing Variables in PIPE

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for the PIPE block.

Block Input

Sentence	Variables	ID1	Element
PARAM	LENGTH, IN-DIAM, ELEVATION, ANGLE, ROUGHNESS, T-OUT, P-OUT, C-EROSION, MAXIT	—	—
METHODS	T-IN, TAMB-IN, TAMB-OUT, H-T-COEFF, FLUX, EFFICIENCY, H-W-COEFF	—	—
TABLE-DEF	TEMP, PRES, TMIN, TMAX, NTEMP, PMIN, PMAX, NPRES, CBAR	—	†
CONVERGENCE	HINIT, INT-TOL, BB1, BB2, BB3, BB4, BB5, BB6, BB7, BB8, BB9, BB10, CDPDL-TOL	—	—
FITTINGS	CONNECTIONS, ELBOWS, STRAIGHT-TEE, BRANCHED-TEE, GATE-VALVES, BUTTERFLY-VA, MISC-L-D, MISC-K, E-ANGLE, E-DIAM, C-ANGLE, C-DIAM, ORIFICE-DIAM, ORIFICE-THIC	—	—

† Position of a value entered for PRES and TEMP in the TABLE-DEF sentence. For other variables, leave element blank.

Block Results

Description	Sentence	Variable	ID1
Flow regime at inlet	RESULTS	IN-REGIME	—
Flow regime at outlet	RESULTS	OUT-REGIME	—
Liquid holdup at inlet	RESULTS	IN-HOLDUP	—
Liquid holdup at outlet	RESULTS	OUT-HOLDUP	—
Velocity at inlet	RESULTS	IN-VELOCITY	—
Velocity at outlet	RESULTS	OUT-VELOCITY	—
Reynolds number at inlet	RESULTS	IN-REYNO	—
Reynolds number at outlet	RESULTS	OUT-REYNO	—
Delta-P due to friction	RESULTS	DP-FRIC	—
Delta-P due to elevation	RESULTS	DP-ELEV	—
Delta-P due to acceleration	RESULTS	DP-ACCEL	—
Total Delta-P	RESULTS	DP-TOTAL	—
Block heat duty	RESULTS	HEAT-DUTY	—
Erosional velocity at inlet	RESULTS	IN-EROVELOC	—
Erosional velocity at outlet	RESULTS	OUT-EROVELOC	—
Liquid volume fractional inlet	RESULTS	IN-LVFRAC	—
Liquid volume fractional outlet	RESULTS	OUT-LVFRAC	—
Vapor volume fraction at inlet	RESULTS	IN-VVFRAC	—
Vapor volume fraction at outlet	RESULTS	OUT-VVFRAC	—
Equivalent length	RESULTS	EQUIV-LENGTH	—

continued

Block Results (continued)

Description	Sentence	Variable	ID1
Temperature	PROFILES	PROF-TEMP	pointno†
Pressure	PROFILES	PROF-PRES	pointno†
Enthalpy	PROFILES	PROF-ENTHALP	pointno†
Density	PROFILES	PROF-DENSITY	pointno†
Reynolds number	PROFILES	PROF-REYNO	pointno†
Velocity	PROFILES	PROF-VELOC	pointno†
Erosional velocity	PROFILES	PROF-EROVEL	pointno†
Ambient temperature	PROFILES	PROF-TAMB	pointno†
Vapor volume fraction	PROFILES	PROF-VFRAC	pointno†
Liquid volume fraction	PROFILES	PROF-LFRAC	pointno†
Liquid superficial velocity	PROFILES	PROF-LVELOC	pointno†
Gas superficial velocity	PROFILES	PROF-GVELOC	pointno†
Liquid mass flow	PROFILES	PROF-LFLOW	pointno†
Gas mass flow	PROFILES	PROF-GFLOW	pointno†
Heat flux	PROFILES	PROF-FLUX	pointno†
Liquid holdup	PROFILES	PROF-HOLDUP	pointno†

† pointno is the profile point number, running sequentially from 1 to NPOINT + 1.

VALVE: Valve Calculation

Input Language for VALVE

```
BLOCK    blockid    VALVE
PARAM    keyword=value
```

Keywords:

P-OUT P-DROP FLO-COEF VAL-POSN

Optional keywords:

NPHASE PHASE CHAR-EQN MAX-FLO-COEF PDROP-FAC PREC-FAC VALVE-DIA IN-PIPE-DIA OUT-PIPE-DIA CHECK-CHOKE CALC-CAVIND CALC-CV MIN-POUT CH-SET-PMIN FLASH-MAXIT FLASH-TOL MAXIT TOL

```
VAL-PARAM    data-no    vp    cv    xt    fl  / . . .
```

Input Language Description for VALVE

PARAM

Use to specify valve operating parameters, calculation options, pipe fitting sizes, flash specifications, and convergence parameters. You must specify one of the following: outlet pressure, pressure drop, valve flow coefficient at operating condition, or percentage valve opening at operating condition.

P-OUT ..... Pressure at valve outlet

P-DROP..... Pressure-drop (inlet - outlet)

FLO-COEF..... Valve flow coefficient at operating condition

VAL-POSN..... Valve opening at operating conditions (as a percentage of maximum opening)

NPHASE ..... Maximum number of phases in inlet and outlet streams:

NPHASE=1	One-phase flash
NPHASE=2	Two-phase flash (Default)
NPHASE=3	Three-phase flash

PHASE..... Phase of inlet and outlet stream when NPHASE=1:

PHASE=V	Vapor
PHASE=L	Liquid (Default)

CHAR-EQN ..... Valve characteristic equation that relates the flow coefficient to the valve opening:

CHAR-EQN=LINEAR	$V = P$
CHAR-EQN=PARABOLIC	$V = 0.01\ P^2$
CHAR-EQN= SQUARE ROOT	$V = 10\sqrt{P}$
CHAR-EQN= QUICK OPENING	$V = \frac{10P}{\sqrt{1 + 9.9 \times 10^{-3} P^2}}$
CHAR-EQN= EQUAL PERCENTAGE	$V = \frac{0.01P^2}{\sqrt{2 - 1 \times 10^{-8} P^4}}$
CHAR-EQN=HYPERBOLIC	$V = \frac{0.1P}{\sqrt{1 - 9.9 \times 10^{-5} P^2}}$

Where:
P = Valve opening as a percentage of maximum opening
V = Flow coefficient as a percentage of flow coefficient at maximum opening

MAX-FLO-COEF ..... Valve flow coefficient at 100% valve opening

PDROP-FAC..... Pressure drop ratio factor for valve. The pressure drop ratio factor accounts for the effect of the valve internal geometry on the change in fluid density as it passes through the valve. (The pressure drop ratio factor is available from valve manufacturer catalogs.)

PREC-FAC..... Pressure recovery factor for valve. The pressure recovery factor accounts for the effect of the valve internal geometry on the liquid flow capacity under choked conditions. (The pressure recovery factor is available from valve manufacturer catalogs.)

VALVE-DIA..... Inlet diameter of valve

IN-PIPE-DIA ..... Diameter of inlet pipe

OUT-PIPE-DIA ..... Diameter of outlet pipe

CHECK-CHOKE..... Option to check for choked flow condition in valve:

CHECK-CHOKE=YES	Checks for choked flow condition (Default)
CHECK-CHOKE=NO	Does not check for choked flow condition

CALC-CAVIND ..... Option to calculate cavitation index for valve:

CALC-CAVIND=YES	Calculates cavitation index
CALC-CAVIND=NO	Does not calculate cavitation index (Default)

CALC-CV..... Option to calculate valve flow coefficient when outlet pressure or pressure drop is specified:

CALC-CV=YES	Calculates valve flow coefficient
CALC-CV=NO	Does not calculate valve flow coefficient. VALVE uses only the keywords P-DROP, P-OUT, NPHASE, PHASE, FLASH-MAXIT, and FLASH-TOL for this option. (Default)

MIN-POUT..... Lower limit on the calculated outlet pressure. Use only when outlet pressure and pressure drop are not specified. (Default=larger value of 1 Pascal and the Plower specification, established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

CH-SET-PMIN..... Option to set the lower limit on the calculated outlet pressure, based on choked flow condition in valve:

CH-SET-PMIN=YES	Sets the lower limit based on the calculated outlet pressure for choked flow
CH-SET-PMIN=NO	Sets the lower limit based on the value established by MIN-POUT (Default)

FLASH-MAXIT ..... Maximum number of iterations for flash calculations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

FLASH-TOL..... Convergence tolerance for flash calculations. (Default=value established by the SIM-OPTIONS paragraph.)
(See Chapter 45.)

MAXIT..... Maximum number of iterations for valve flow coefficient calculations (Default=50)

TOL ..... Convergence tolerance for valve flow coefficient calculations (Default=$1x10^{-4}$)

VAL-PARAM

Use to specify data for valve parameters (flow coefficient, pressure drop ratio factor, and pressure recovery factor), for varying valve positions.

data-no..... Entry number (sequential, starting at 1)

vp ..... Data for valve position as a percentage of maximum opening (in increasing order)

cv..... Data for valve flow coefficient

xt..... Data for pressure drop ratio factor. The pressure drop ratio factor accounts for the effect of the valve internal geometry on the change in fluid density as it passes through the valve. (The pressure drop ratio factor is available from valve manufacturer catalogs.)

fl..... Data for pressure recovery factor. The pressure recovery factor accounts for the effect of the valve internal geometry on the liquid flow capacity under choked conditions. (The pressure recovery factor is available from valve manufacturer catalogs.)

Accessing Variables in VALVE

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1
PARAM	VAL-POSN, P-OUT, P-DROP, FLO-COEF, MAX-FLO-COEF, PDROP-FAC, PREC-FAC, VALVE-DIA, IN-PIPE-DIA, OUT-PIPE-DIA, MAXIT, TOL, FLASH-MAXIT, FLASH-TOL	—
VAL-PARAM	VP, CV, XT, FL	data-no

Block Results

Description	Sentence	Variable
Calculated valve outlet pressure	RESULTS	P-OUT-R
Calculated valve flow coefficient†	RESULTS	FLO-COEF-R
Calculated valve pressure drop	RESULTS	P-DROP-R
Calculated percentage valve opening†	RESULTS	VAL-POSN-R
Valve outlet pressure for choked flow condition	RESULTS	CHOKE-POUT
Valve cavitation index	RESULTS	CAV-IND
Expansion factor (ratio of valve flow coefficient for a gas, to that of a liquid at the same Reynolds number)	RESULTS	EXP-FAC
Pressure recovery factor for the valve†	RESULTS	FL-FAC
Pressure drop ratio factor for the valve†	RESULTS	XT-FAC
Ratio of specific heats factor	RESULTS	FK-FAC
Liquid critical pressure ratio factor	RESULTS	FF-FAC
Piping geometry factor (ratio of flow coefficient for a valve with attached fittings, to that for a valve installed in a straight pipe of the same size as the valve)	RESULTS	FP-FAC
Pressure recovery factor for a valve with attached pipe fittings†	RESULTS	FLP-FAC
Pressure drop ratio factor for a valve with attached pipe fittings†	RESULTS	XTP-FAC

† At operating valve opening.

22 Crystallizer

This chapter describes the input language for the crystallization model. The model is:

Model	Description	Purpose	Use
CRYSTALLIZER	Continuous crystallizer	Forms crystal from solution based on equilibrium calculations	Steady state crystallization, precipitation, and evaporation

CRYSTALLIZER: Continuous Crystallizer

Input Language for CRYSTALLIZER

```
BLOCK    blockid    CRYSTALLIZER
PARAM    keyword=value
```

Keywords:

SOL-METHOD TEMP PRES DUTY PROD-RATE basis-VFLOW

Optional keywords:

FRAC-RFLOW basis-RFLOW HEATER-DELT PSD-FLAG NPHASE VOL SALT SALT-IN SALT-OUT SOL-BASIS SOLVENT-CID FRAC-COV MAXIT TOL TUPPER TLOWER TOL-RATIO MAX-TSTEP TEAR-METHOD DS-ITERS QMAX QMIN FLASH-MAXIT FLASH-TOL T-EST P-EST

```
STOIC    reacno    ssid    cid    coef / cid    coef / ...
SOLU-PROFILE    solub-temp    solub-concen    [solub-ratio] / ...
RATE-PARAMS    keyword=value
```

Keyword:

KBO

Optional keywords:

BNI BNJ BNK GAMMA ALPHA

```
AGITATOR    RATE=value
CRYSTAL    VOLUME-SHAPE=value
COMP-ATTR    entryno    ssid    cid    cattrname    (value)
SUBS-ATTR    entryno    ssid    psdid    (value)
SUBROUTINE    SOLUBILITY=subrname
SOL-VECS    keyword=value
```

Keywords:

NSINT NSREAL NIWORKS NWORKS

```
SINT    value-list
SREAL    value-list
```

Input Language Description for CRYSTALLIZER

PARAM

Use to specify operating conditions.

SOL-METHOD ..... Calculation method to determine the saturation concentration:

SOL-METHOD= SOLUBILITY	Calculates crystal product from a solubility curve provided by the SOLU-PROFILE sentence (Default)
SOL-METHOD= CHEMISTRY	Calculates crystal product based on electrolyte chemistry

	SOL-METHOD=USER-SUBR	Calculates crystal product based on user-provided FORTRAN subroutine for saturation concentration. You can also use the subroutine to calculate crystal product directly.
TEMP	Crystallizer temperature	
PRES	**PRES > 0**	Crystallizer pressure
	PRES ≤ 0	Pressure drop between outlet and inlet streams
DUTY	Heat duty applied to heat exchanger	
PROD-RATE	Crystal product flow rate	
basis-VFLOW	Vapor flow rate in MOLE, MASS, and STDVOL basis	
FRAC-RFLOW	Fraction of outlet flow from crystallizer being recycled	
basis-RFLOW	Recirculation flow rate in MOLE, MASS, and STDVOL basis	
HEATER-DELT	Temperature change across heat exchanger	
PSD-FLAG	**PSD-FLAG=YES**	Determines crystal particle size distribution
	PSD-FLAG=NO	Does not determine crystal particle size distribution (Default)
NPHASE	**NPHASE=1**	One-phase calculation
	NPHASE=2	Two-phase flash (Default)
VOL	Crystallizer volume	
SALT	Component ID of crystallizing salt if SOL-METHOD=CHEMISTRY	
SALT-IN	**SALT-IN=YES**	Moves crystallizing salt from the first CI (conventional inert) solids substream of inlet stream when SOL-METHOD=CHEMISTRY (Default)
	SALT-IN=NO	Does not move crystallizing salt from the first CI solids substream of inlet stream when SOL-METHOD=CHEMISTRY
SALT-OUT	**SALT-OUT=YES**	Moves crystallizing salt to the first CI solids substream of product stream when SOL-METHOD=CHEMISTRY (Default)
	SALT-OUT=NO	Does not move crystallizing salt to the first CI solids substream of product stream when SOL-METHOD=CHEMISTRY
SOL-BASIS	Basis of solubility data:	
	SOL-BASIS=SOLUTION	Solubility data expressed in terms of mass of solute per unit volume (or mass) of solution
	SOL-BASIS=SOLVENT	Solubility data expressed in terms of mass of solute per unit volume (or mass) of solvent
SOLVENT-CID	Solvent component ID if SOL-BASIS=SOLVENT	
FRAC-COV	Fractional coefficient of variation for reporting crystal PSD (Default=0.16)	
MAXIT	Maximum iterations for all calculations, except flash convergence (Default=50)	
TOL	Tolerance for all calculations, except flash convergence (Default=$1x10^{-4}$)	
TUPPER	Upper bound of temperature iteration	
TLOWER	Lower bound of temperature iteration	
TOL-RATIO	Ratio of inner loop tolerance to outer loop tolerance (Default=0.1)	

MAX-TSTEP ..... Maximum temperature step for temperature iteration (Default=10 K)

TEAR-METHOD ..... Method to converge the tear stream if there is a recycled stream:

TEAR-METHOD= BROYDEN	Broyden method (Default)
TEAR-METHOD= WEGSTEIN	Bounded Wegstein method
TEAR-METHOD=DIRECT	Direct substitution method

DS-ITERS ..... Number of steps using direct substitution before changing to Broyden or Wegstein method (Default=3)

QMAX ..... Maximum value of bounded Wegstein acceleration parameter for tear stream (Default=0.5)

QMIN ..... Minimum value of bounded Wegstein acceleration parameter for tear stream (Default=-20)

FLASH-MAXIT ..... Maximum iterations for flash convergence. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

FLASH-TOL ..... Flash convergence tolerance. Defaults to the minimum value of TOL/(10*TOL-RATIO) and the global flash tolerance. (Global flash tolerance is established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

T-EST ..... Temperature estimate. Use to aid flash convergence when TEMP is not specified.

P-EST ..... Pressure estimate. Use to aid flash convergence when PRES is not specified.

STOIC Use to enter the stoichiometry of crystal formation.

reacno ..... Reaction number (must be 1)

ssid ..... Substream ID

cid ..... Component ID

coef ..... Stoichiometric coefficient (positive for products; negative for reactants). For nonconventional components, the coefficient is the mass of the generated component.

SOLU-PROFILE Use to specify the solubility data if SOL-METHOD=SOLUBILITY.

solub-temp ..... Solubility temperature

solub-concen ..... Solubility data. Defines mass of solute per unit volume of solution or solvent.

solub-ratio ..... Solubility data. Defines mass of solute per unit mass of solution or solvent.

RATE-PARAMS Use to enter the overall nucleation rate, and coefficients for size-dependent growth rate.

KBO ..... Overall nucleation rate coefficient

BNI ..... Exponent in overall nucleation rate for growth rate term (Default=1)

BNJ ..... Exponent in overall nucleation rate for magma density term (Default=1)

BNK ..... Exponent in overall nucleation rate for agitator rotation rate term (Default=0)

	GAMMA	Coefficient for size-dependent growth rate (Default=0)
	ALPHA	Exponent for size-dependent growth rate (Default=0)
AGITATOR	Use to enter the impeller rotation rate.	
	RATE	Impeller tip rotation rate (Default=0 rev/s)
CRYSTAL	Use to describe the crystal characteristics.	
	VOLUME-SHAPE	Volume shape factor of the crystal (Default=1.0 for cubic crystals)
COMP-ATTR	Use to specify outlet stream values of component attributes created or changed by crystallization. Enter one COMP-ATTR sentence for each component attribute.	
	entryno	Entry number
	ssid	Substream ID
	cid	Component ID
	cattrname	Component attribute name
	value	List of attribute values to be entered or changed. You should insert an asterisk (*) for values not changed.
SUBS-ATTR	Use to specify outlet stream values of the particle-size distribution for a substream created or changed by crystallization. Enter one SUBS-ATTR sentence for each substream. To specify the SUBS-ATTR sentence and bypass system calculation of particle-size distribution, you must set PSD-FLAG=NO.	
	entryno	Entry number
	ssid	Substream ID
	psdid	Particle size distribution ID
	value	List of attribute values to be entered or changed. You should insert an asterisk (*) for values not changed.
SUBROUTINE	Use to specify user-supplied solubility subroutine. For details on writing user-supplied solubility subroutines, see *Aspen Plus User Models*, Chapter 23.	
	SOLUBILITY	User-supplied FORTRAN subroutine name for providing saturation concentration of crystal product calculation, or for calculating crystal product.
SOL-VECS	Use to define the length of arrays for the user-supplied solubility subroutine.	
	NSINT	Length of integer parameter array
	NSREAL	Length of real parameter array
	NIWORKS	Length of integer workspace array
	NWORKS	Length of real workspace array
SINT	Use to enter values for the integer parameter array of the user-supplied solubility subroutine.	
	value-list	List of integer values
SREAL	Use to enter values for the real parameter array of the user-supplied solubility subroutine.	
	value-list	List of real values

Accessing Variables in CRYSTALLIZER

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for a CRYSTALLIZER block.

Block Input

Sentence	Variables	ID1	ID2	ID3	Element
PARAM	TEMP, PRES, DUTY, PROD-RATE, basis-VFLOW, FRAC-RFLOW, basis-RFLOW, HEATER-DELT, VOL, FRAC-COV, MAXIT, TOL, QMAX, QMIN, MAX-TSTEP, TUPPER, TLOWER, T-EST, P-EST	—	—	—	—
STOIC	COEF	1	ssid	cid	—
COMP-ATTR	VALUE	entryno	—	—	†
SUBS-ATTR	VALUE	entryno	—	—	†
SINT	VALUE-LIST	—	—	—	†
SREAL	VALUE-LIST	—	—	—	†
RATE-PARAMS	KBO, BNI, BNJ, BNK, GAMMA, ALPHA	—	—	—	—
AGITATOR	RATE	—	—	—	—
CRYSTAL	VOLUME-SHAPE	—	—	—	—

† Position of a value in the COMP-ATTR, SUBS-ATTR, SINT, or SREAL value-list.

Block Results

Description	Sentence	Variable
Heat duty	PARAM	QCALC
Temperature	PARAM	TCALC
Pressure	PARAM	PCALC
Residence time	RESULT-CRYST	TIME-CAL
Product flow rate	RESULT-CRYST	PRATE-CAL
Vent flow rate	RESULT-CRYST	VENT-CAL
Recycled flow	RESULT-CRYST	REC-FLOW
Magma density	RESULT-CRYST	MT-CAL
Growth rate	RESULT-CRYST	G-CAL
Nucleation rate	RESULT-CRYST	BO-CAL
Mean size	RESULT-CRYST	MEAN-SIZE
Standard deviation	RESULT-CRYST	STAND-DEV
Skewness	RESULT-CRYST	SKEWNESS
Coefficient of variance	RESULT-CRYST	COEFF-VAR
Zeroth moment	RESULT-CRYST	MOMENT0
First moment	RESULT-CRYST	MOMENT1
Second moment	RESULT-CRYST	MOMENT2
Third moment	RESULT-CRYST	MOMENT3
Fourth moment	RESULT-CRYST	MOMENT4
Net heat duty	RESULT-CRYST	NET-DUTY

23 Crushers and Screens

This chapter describes the input language for models that break and separate solid particles. The models are:

Model	Description	Purpose	Use
CRUSHER	Solids crusher	Breaks solid particles to reduce particle size	Wet and dry crushers, primary and secondary crushers
SCREEN	Solids separator	Separates solid particles based on particle size	Upper and lower dry and wet screens

CRUSHER: Solids Crusher

Input Language for CRUSHER

```
BLOCK    blockid    CRUSHER
PARAM    keyword=value
```

Keyword:

DIAM

Optional keywords:

MODE TYPE RATIO-CUT

```
BWI    ssid    bwl  /  ...
HGI    ssid    hgi  /  ...
SELECT-FUN    size-ratio    value  /  ...
BREAK-FUN    size-ratio    value  /  ...
BCUT-FUN    size-ratio    value  /  ...
```

Input Language Description for CRUSHER

PARAM

Use to enter crusher parameters. You must specify the maximum diameter of particles in the crusher outlet. You can also specify the mode of operation and the type of crusher.

DIAM	Maximum diameter of particles in the crusher outlet	
MODE	**MODE=PRIMARY**	Primary operating mode (Default)
	MODE=SECONDARY	Secondary operating mode
TYPE	Crusher type:	
	TYPE=GYRATORY	Gyratory jaw (Default)
	TYPE=SINGLE-ROLE	Single-roll
	TYPE=MULTIPLE-ROLL	Multiple-roll
	TYPE=CAGE-MILL	Cage-mill
RATIO-CUT	Ratio of cut-off size to solids diameter, which determines the breakage function to be used (Default=1.7)	

BWI

Use to enter the Bond work index for each solids substream being crushed. You cannot use BWI if you specified HGI.

ssid	Substream ID
bwi	Bond work index for the specified solids substream. Use UNITS keyword BOND-WORK-INDEX to specify units.

HGI

Use to enter the Hardgrove grindability index for each solids substream being crushed. You cannot use HGI if you specified BWI.

ssid	Substream ID
hgi	Hardgrove grindability index for the specified solids substream. Use UNITS keyword BOND-WORK-INDEX to specify units.

SELECT-FUN

Use to specify the selection function as a function of ratio of feed size to outlet diameter. If you do not provide SELECT-FUN, CRUSHER uses the built-in selection based on operating mode.

size-ratio	Ratio of feed size to outlet diameter

value..... Value of selection function for crusher

BREAK-FUN Use to specify the breakage function as a function of ratio of product size to feed size when feed size is greater than cut-off size. Cut-off size equals RATIO-CUT*DIAM. If you do not provide BREAK-FUN, CRUSHER uses the built-in breakage function based on crusher type.

size-ratio ..... Ratio of product size to feed size

value..... Value of breakage function for particle size greater than cut-off size

BCUT-FUN Use to specify the natural breakage function as a function of ratio of product size to feed size when feed size is less than cut-off size. Cut-off size equals RATIO-CUT*DIAM. If you do not provide BCUT-FUN, CRUSHER uses the built-in natural breakage function.

size-ratio ..... Ratio of product size to feed size

value..... Value of natural breakage function for particle size less than cut-off size

Accessing Variables in CRUSHER

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for a CRUSHER block.

Block Input

Sentence	Variable	ID1
PARAM	DIAM	—
BWI	BWI	ssid
HGI	HGI	ssid

Block Results

Description	Sentence	Variable
Power required	PARAM	POWER

SCREEN: Solid Particle Separator

Input Language for SCREEN

```
BLOCK    blockid    SCREEN
PARAM    keyword=value
```

Keyword:

OPENING

Optional keywords:

LEVEL MODE STRENGTH ENTRN

```
SEP-STRENGTH    size    value  / ...
SELECT-FUN    diam    value  / ...
```

Input Language Description for SCREEN

PARAM

Use to specify screen parameters. You must specify the size of the screen opening. You can also specify the operating level, the mode of operation, and the separation strength of the screen.

OPENING	Size of screen opening	
LEVEL.....	**LEVEL=UPPER**	Upper operating level (Default)
	LEVEL=LOWER	Lower operating level
MODE.....	**MODE=DRY**	Dry operating mode
	MODE=WET	Wet operating mode (Default is determined from inlet stream vapor fraction. If vapor fraction is 1, dry operation is assumed. Otherwise, wet operation is assumed.)
STRENGTH	Separation strength of the screen. You cannot use STRENGTH if you specified SEP-STRENGTH or SELECT-FUN. (Default is a function of screen opening.)	
ENTRN	Fraction of components in the mixed substream of feed stream entrained in the overflow of the outlet stream. (Default=0)	

SEP-STRENGTH

Use to specify the separation strength as a function of size of screen opening. You cannot use SEP-STRENGTH if you specified SELECT-FUN or keyword STRENGTH in the PARAM sentence.

size.....	Size of screen opening
value.....	Value for screen separation strength

SELECT-FUN

Use to specify the selection function as a function of particle size. You cannot use SELECT-FUN if you specified SEP-STRENGTH or keyword STRENGTH in the PARAM sentence.

diam	Particle diameter
value.....	Value for screen selection function

Accessing Variables in SCREEN

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for a SCREEN block.

Block Input

Sentence	Variables
PARAM	OPENING, STRENGTH, ENTRN

Block Results

Description	Sentence	Variable
Calculated efficiency	RESULTS	EFF
Calculated separation strength	RESULTS	SEP-STRENGTH
Determined mode (0=DRY, 1=WET)	RESULTS	MODE

24 Gas-Solid Separators

This chapter describes the input language for models that separate solids from a gas stream. The models are:

Model	Description	Purpose	Use
FABFL	Fabric filter	Separate solids from gas using fabric filter baghouses	Rating and sizing baghouses
CYCLONE	Cyclone separator	Separate solids from gas using gas vortex in a cyclone	Rating and sizing cyclones
VSCRUB	Venturi scrubber	Separate solids from gas by direct contact with an atomized liquid	Rating and sizing venturi scrubbers
ESP	Electrostatic precipitator	Separate solids from gas using an electric charge between two plates	Rating and sizing dry electrostatic precipitators

FABFL: Fabric Filter

Input Language for FABFL

```
BLOCK    blockid    FABFL
PARAM    keyword=value
```

Optional keywords:

MODE CALCULATE RESISTANCE COPY-PRES

```
BAG-PROPS    keyword=value
```

Keyword:

NCELLS

Optional keywords:

NCLEAN NBAGS DIAM AREA PDROP

```
OPERATION    keyword=value
```

Keywords:

MAX-PDROP FILT-TIME

Optional keywords:

CLEAN-TIME MAX-VEL MIN-VEL INIT-VEL

```
EFFICIENCY    diam    eff  /  ...
```

Input Language Description for FABFL

PARAM Use to enter calculation mode, options, and dust resistance coefficient.

MODE	**MODE=SIMULATION**	Performs simulation mode calculations (Default)
	MODE=DESIGN	Performs design mode calculations
CALCULATE	**CALCULATE=TIME**	Calculates time of filtration (Default)
	CALCULATE=PRESSURE	Calculates pressure drop
RESISTANCE	Dust resistance coefficient for filtration. Units must be in $Pa/(kg/m^2)/(m/s)$. (Default=60000 $Pa/(kg/m^2)/(m/s)$)	
COPY-PRES	**COPY-PRES = YES**	Outlet solids stream pressure is the same as inlet gas-solids stream pressure
	COPY-PRES = NO	Outlet solids stream pressure is the same as outlet gas-solids stream pressure (Default)

BAG-PROPS Use to specify baghouse characteristics.

NCELLS	Number of cells. Use only when MODE=SIMULATION.
NCLEAN.....	Number of cells being cleaned (Default=1)
NBAGS	Number of bags per cell (Default=78)
DIAM	Diameter of a bag (Default=0.154 m)
AREA.....	Filtering area per bag (Default=1.48 m^2)
PDROP	Pressure drop of the clean bag (Default=250 N/m^2)

OPERATION Use to specify filter operating conditions.

MAX-PDROP	Maximum allowable pressure drop. Use only when CALCULATE=TIME.
FILT-TIME	Time of filtration. Use only when CALCULATE=PRESSURE.
CLEAN-TIME	Time required to clean the bags (Default=30 sec)
MAX-VEL	Maximum allowable velocity of the gas through the cloth of the bags in the baghouse (Default=0.0254 m/sec)
MIN-VEL	Minimum allowable velocity of the gas through the cloth of the bags in the baghouse (Default=0.00254 m/sec)
INIT-VEL	Initial estimate of the velocity of the gas through the cloth for the design option. Use only when MODE=DESIGN. (Default=0.015 m/sec)

EFFICIENCY Use to specify the efficiency table as a function of particle sizes.

diam	Diameter of solid particles to be separated
eff	Collection efficiency of solid particles of the baghouse

Accessing Variables in FABFL

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for a FABFL block.

Block Input

Sentence	Variables
PARAM	RESISTANCE
BAG-PROPS	NCELLS, NCLEAN, NBAGS, DIAM, AREA, PDROP
OPERATION	MAX-PDROP, FILT-TIME, CLEAN-TIME, MAX-VEL, MIN-VEL, INIT-VEL

Block Results

Description	Sentence	Variable
Collection efficiency	RESULTS	EFF
Number of cells	RETENTION	NCELLS

CYCLONE: Cyclone Separator

Input Language for CYCLONE

```
BLOCK    blockid    CYCLONE
PARAM    keyword=value
```

Optional keywords:

MODE METHOD TYPE VANE MAXIT TOL

DESIGN *keyword=value*

Keyword:

EFF

Optional keywords:

MAX-CYCLONE MAX-PDROP

SIMULATION *keyword=value*

Keyword:

DIAM

Optional keyword:

NCYCLONE

DIMENSIONS *keyword=value*

Keywords:

LEN-CYLINDER LEN-CONE DIAM-OVER LEN-OVER WIDTH-INLET HT-INLET DIAM-UNDER

Optional keyword:

NTURN

RATIOS *keyword=value*

Keywords:

LEN-CYLINDER LEN-CONE DIAM-OVER LEN-OVER WIDTH-INLET HT-INLET DIAM-UNDER

Optional keywords:

NTURN MAX-DIAM

EFFICIENCY [diam] [eff] / ... **SOL-LOADING** *keyword=value*

Optional keywords:

CR-SOL-LOAD EFF-CON1 PRES-CON1 PRES-CON2

Input Language Description for CYCLONE

PARAM Use to enter calculation mode and options, type of cyclone, and vane constant.

MODE	**MODE=SIMULATION**	Performs simulation mode calculations (Default)
	MODE=DESIGN	Performs design mode calculations
METHOD	**METHOD=LEITH-LICHT**	Uses the Leith-Licht efficiency correlation (Default)
	METHOD=LAPPLE	Uses the Shepherd and Lapple efficiency correlation
	METHOD= MOD-LEITH-LICHT	Uses modified Leith-Licht correlation
	METHOD=DIETZ	Uses Dietz efficiency correlation
	METHOD=MOTHES-LOF	Uses Mothes and Loffler efficiency correlation
	METHOD=USER	Uses a user-specified efficiency curve
TYPE	**TYPE=HIGH**	High efficiency (Default)

	TYPE=MEDIUM	Medium efficiency
	TYPE=USER	User-specified cyclone dimensions. Allowed only when MODE=SIMULATION.
	TYPE=USER-RATIO	User-specified dimension ratios
VANE		Vane constant used in pressure drop equation of Shepherd and Lapple. You must specify METHOD=LAPPLE. (Default=16)
MAXIT		Maximum number of iterations for determining the cyclone diameter in DESIGN mode (Default=30)
TOL		Convergence tolerance for determining the cyclone diameter in DESIGN mode (Default=$1x10^{-4}$)

DESIGN Use to enter parameters for design mode calculations. You cannot use DESIGN if you specified SIMULATION.

EFF	Efficiency
MAX-CYCLONE	Maximum number of cyclones in parallel (Default=100)
MAX-PDROP	Maximum allowable pressure drop. If the pressure drop exceeds this limit, several smaller cyclones in parallel will be designed. (Default=1500 N/m^2)

SIMULATION Use to enter parameters for simulation mode calculations. You cannot use SIMULATION if you specified DESIGN.

DIAM	Diameter of the cyclone
NCYCLONE	Number of cyclones. If NCYCLONE > 1, cyclones are in parallel. (Default=1)

DIMENSIONS Use to specify cyclone dimensions when MODE=SIMULATION and TYPE=USER.

LEN-CYLINDER	Length of cylinder
LEN-CONE	Length of cone section
DIAM-OVER	Diameter of overflow
LEN-OVER	Length of overflow
WIDTH-INLET	Width of inlet
HT-INLET	Height of inlet
DIAM-UNDER	Diameter of underflow
NTURN	Number of gas turns in the cyclone (Default=5.5)

RATIOS Use to specify the ratios of a cyclone dimension to the cyclone diameter when TYPE=USER-RATIO.

LEN-CYLINDER	Ratio of length of cylinder to cyclone diameter
LEN-CONE	Ratio of length of cone section to cyclone diameter
DIAM-OVER	Ratio of diameter of overflow to cyclone diameter
LEN-OVER	Ratio of length of overflow to cyclone diameter
WIDTH-INLET	Ratio of width of inlet to cyclone diameter
HT-INLET	Ratio of height of inlet to cyclone diameter
DIAM-UNDER	Ratio of diameter of underflow to cyclone diameter
NTURN	Number of gas turns in the cyclone (Default=5.5)
MAX-DIAM	Maximum allowable diameter of the cyclone (Default=3.0 m)

EFFICIENCY Use to specify the efficiency table as a function of particle sizes when METHOD=USER.

diam ..... Diameter of solid particles to be separated

eff ..... Collection efficiency of solid particles to be separated

SOL-LOADING Use to specify constants for correlations that correct the pressure drop and cyclone efficiency based on the presence of solids in the gas flow.

CR-SOL-LOAD..... Critical solids loading in the feed above which the cyclone efficiency and pressure drop are affected (Default=$1x10^{-3}$ kg/m^3)

EFF-CON1..... Exponent in the correlation that adjusts the cyclone efficiency due to solids loading

PRES-CON1 ..... Pre-exponential factor in the correlation that adjusts the pressure drop due to solids loading. You must also specify PRES-CON2.

PRES-CON2 ..... Exponent in the correlation that adjusts the pressure drop due to solids loading. You must also specify PRES-CON1.

Accessing Variables in CYCLONE

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for a CYCLONE block.

Block Input

Sentence	Variables
PARAM	VANE
DESIGN	EFF, MAX-CYCLONE, MAX-PDROP
SIMULATION	DIAM, NCYCLONE
DIMENSIONS	LEN-CYLINDER, LEN-CONE, DIAM-OVER, LEN-OVER, WIDTH-INLET, HT-INLET, DIAM-UNDER, NTURN
RATIOS	LEN-CYLINDER, LEN-CONE, DIAM-OVER, LEN-OVER, WIDTH-INLET, HT-INLET, DIAM-UNDER, NTURN, MAX-DIAM
SOL-LOADING	CR-SOL-LOAD, EFF-CON1, PRE-CON1, PRE-CON2

Block Results

Description	Sentence	Variable
Calculated efficiency	RESULTS	EFF
Calculated vortex length	RESULTS	VORTEX-LENGTH
Calculated diameter	DIMENSIONS	DIAM
Ratio of inlet to saltation velocity	RET-SCALAR	VEL-RATIO

VSCRUB: Venturi Scrubber

Input Language for VSCRUB

```
BLOCK    blockid    VSCRUB
SIMULATION    keyword=value
```

Keywords:

DIAM-THROAT LEN-THROAT

```
DESIGN    keyword=value
```

Keyword:

EFF

Optional keyword:

VOL-RATIO

```
OPERATION    keyword=value
```

Optional keywords:

MAX-VEL MIN-VEL MAX-RATIO MIN-RATIO MAX-DIAM MIN-DIAM LIQ-VEL OUTLT-EQUIL

Input Language Description for VSCRUB

SIMULATION Use to enter parameters for simulation mode calculations. You must specify both DIAM-THROAT and LEN-THROAT. You cannot use SIMULATION if you specified DESIGN.

DIAM-THROAT ..... Diameter of the throat of the venturi scrubber

LEN-THROAT ..... Length of the throat of the venturi scrubber

DESIGN Use to enter parameters for design mode calculations. You must specify EFF. You cannot use DESIGN if you specified SIMULATION.

EFF..... Separation efficiency. Defined as the ratio of the mass flow rate of the solid particles in the outlet liquid stream to the mass flow rate of the particles in the inlet gas stream.

VOL-RATIO ..... Initial guess for the volume ratio of liquid to gas (Default=0.001)

OPERATION Use to specify optional operating conditions and parameters.

MAX-VEL ..... Maximum gas velocity allowed at the throat (Default=120 m/s)

MIN-VEL ..... Minimum velocity allowed at the throat (Default=50 m/s)

MAX-RATIO..... Maximum volume ratio of liquid-flow rate to gas-flow rate allowed (Default=0.0016)

MIN-RATIO ..... Minimum volume ratio of liquid-flow rate to gas-flow rate allowed (Default=0.000668)

MAX-DIAM ..... Maximum value allowed for the diameter of the throat (Default=1.15 m)

MIN-DIAM..... Minimum value allowed for the diameter of the throat (Default=0.15 m)

LIQ-VEL ..... Entering velocity of the liquid at the throat (Default=0 m/s)

OUTLT-EQUIL..... Whether VSCRUB ensures that its exit streams reach equilibrium at constant total enthalpy by performing PQ flash.

OUTLT-EQUIL=YES	Exit streams reach equilibrium (Default)
OUTLT-EQUIL=NO	Exit streams do not reach equilibrium. Exit liquid and vapor stream temperatures and their mixed substream flowrates and compositions are held at inlet values.

Accessing Variables in VSCRUB

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for a VSCRUB block.

Block Input

Sentence	Variables
SIMULATION	DIAM-THROAT, LEN-THROAT
DESIGN	EFF, VOL-RATIO
OPERATION	MAX-VEL, MIN-VEL, MAX-RATIO, MIN-RATIO, MAX-DIAM, MIN-DIAM, LIQ-VEL

Block Results

Description	Sentence	Variable
Efficiency	RESULTS	EFF
Pressure drop	RESULTS	PDROP
Drop diameter	RESULTS	DROP-DIAM
Gas velocity	RESULTS	GAS-VEL
Throat diameter	RESULTS	DIAM-THROAT
Throat length	RESULTS	LEN-THROAT

ESP: Electrostatic Precipitator

Input Language for ESP

```
BLOCK    blockid    ESP
SIMULATION    keyword=value
```

Keywords:

NPLATE HT-PLATE LEN-PLATE

```
DESIGN    keyword=value
```

Keyword:

EFF

Optional keywords:

GAS-VEL MAX-HT MIN-LEN MAX-LEN MAX-WIDTH

```
WIRE-SPECS    keyword=value
```

Optional keywords:

PLATE-WIRE WIRE-WIRE DIAM

```
OPERATION    keyword=value
```

Optional keywords:

ROUGHNESS MIN-VEL MAX-VEL STDDEV-VEL VOLT-BREAK

```
DIELECTRIC    ssid    dielec  /  ...
```

Input Language Description for ESP

SIMULATION Use to enter parameters for simulation mode calculations. You must specify all parameters. You cannot use SIMULATION if you specified DESIGN.

NPLATE ..... Number of plates in the precipitator

HT-PLATE ..... Height of the plate

LEN-PLATE ..... Length of the plate

DESIGN Use to enter parameters for design mode calculations. You must specify the separation efficiency. You cannot use DESIGN if you specified SIMULATION.

EFF..... Separation efficiency

GAS-VEL..... Initial estimate of the gas velocity (Default=2 m/s)

MAX-HT..... Maximum height of the plate (Default=8.4 m)

MIN-LEN ..... Minimum length of the plate (Default=0.1 m)

MAX-LEN..... Maximum length of the plate (Default=6.3 m)

MAX-WIDTH..... Maximum width of precipitator (Default=8.4 m)

WIRE-SPECS Use to specify optional dimensions of the precipitator.

PLATE-WIRE ..... Distance between the plate and the wire (Default=0.114 m)

WIRE-WIRE ..... Distance between two adjacent wires (Default=0.15 m)

DIAM ..... Diameter of the wire (Default=0.003 m)

OPERATION Use to specify optional operating conditions and parameters.

ROUGHNESS..... Roughness factor of the wire (Default=0.6)

MIN-VEL ..... Minimum allowable gas velocity (Default=0.5 m/s)

MAX-VEL ..... Maximum allowable gas velocity (Default=3 m/s)

STDDEV-VEL ..... Relative standard deviation of gas velocity along the plates (Default=0.15)

VOLT-BREAK ..... Breakdown voltage of the gas in uniform field (Default=3,000,000V)

DIELECTRIC Use to enter the dielectric constants of the solids substreams.

ssid ..... Solids substream ID

dielec ..... Dielectric constant for the substream

Accessing Variables in ESP

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for an ESP block.

Block Input

Sentence	Variables	ID1
SIMULATION	NPLATE, HT-PLATE, LEN-PLATE	—
DESIGN	EFF, GAS-VEL, MAX-HT, MIN-LEN, MAX-LEN, MAX-WIDTH	—
WIRE-SPECS	PLATE-WIRE, WIRE-WIRE, DIAM	—
OPERATION	ROUGHNESS, MIN-VEL, MAX-VEL, STDDEV-VEL, VOL-BREAK	—
DIELECTRIC	DIELEC	ssid

Block Results

Description	Sentence	Variable
Efficiency	RESULTS	EFF
Corona voltage	RESULTS	VOLT-CORONA
Power	RESULTS	POWER
Pressure drop	RESULTS	PDROP
Gas velocity	RESULTS	GAS-VEL
Plate height	RESULTS	HT-PLATE
Plate length	RESULTS	LEN-PLATE

25 Liquid-Solid Separators

This chapter describes the input language for models that separate liquids from solids. The models are:

Model	Type	Purpose	Use
HYCYC	Hydrocyclone	Separate solids from liquid using liquid vortex in a hydrocyclone	Rating or sizing hydrocyclones
CFUGE	Centrifuge filter	Separate solids from liquid using a rotating basket	Rating or sizing centrifuges
FILTER	Rotary vacuum filter	Separate solids from liquid using a continuous rotary vacuum filter	Rating or sizing rotary vacuum filters
DRYER	Solids dryer	Separate solids from liquid by drying	All types of solids dryers

HYCYC: Hydrocyclone

Input Language for HYCYC

```
BLOCK    blockid    HYCYC
SIMULATION    keyword=value
```

Keyword:

DIAM

Optional keyword:

NCYCLONE

```
DESIGN    keyword=value
```

Keywords:

DIAM-PART EFF MAX-DIAM MAX-PDROP

Optional keyword:

DEN-PART

```
RATIOS    keyword=value
```

Optional keywords:

INLET LENGTH OVER UNDER CONE-ANGLE

```
COEFFICIENTS    keyword=value
```

Optional keywords:

VEL-COEF VEL-EXP VOL-RATIO

```
EFFICIENCY    diam    eff  / . . .
```

Input Language Description for HYCYC

SIMULATION Use to enter parameters for simulation mode calculations. You must specify the hydrocyclone diameter. You cannot use SIMULATION if you specified DESIGN.

DIAM	Hydrocyclone diameter
NCYCLONE	Number of hydrocyclones. If NCYCLONE > 1, hydrocyclones are in parallel. (Default=1)

DESIGN Use to enter parameters for design mode calculations. You must specify the diameter of solid particles, the separation efficiency, the maximum diameter of the hydrocyclone, and maximum pressure drop. You cannot use DESIGN if you specified SIMULATION.

DIAM-PART	Diameter of solid particles to be separated
EFF.....	Separation efficiency of solid particles to be separated
MAX-DIAM	Maximum diameter of the hydrocyclone
MAX-PDROP.....	Maximum pressure drop allowed
DEN-PART	Density of solid particles to be separated (Default=density of solids in the inlet solids stream)

RATIO Use to enter optional parameters for the ratios of hydrocyclone dimensions to hydrocyclone diameter. You can also enter cone angle.

- **INLET** ..... Ratio of the inlet diameter to the hydrocyclone diameter (Default=1/7)
- **LENGTH** ..... Ratio of the length to the diameter of the hydrocyclone (Default=5)
- **OVER** ..... Ratio of the overflow diameter to the hydrocyclone diameter (Default=0.2)
- **UNDER** ..... Ratio of the underflow diameter to the hydrocyclone diameter (Default=0.15)
- **CONE-ANGLE** ..... Cone angle of the hydrocyclone (Default=0.349 radians or 20°)

COEFFICIENTS Use to enter optional parameters for the tangential velocity correlation and the ratio of volumetric flows.

- **VEL-COEF** ..... Inlet velocity loss coefficient (Default=0.45)
- **VEL-EXP** ..... Exponent of radial dependence (Default=0.8)
- **VOL-RATIO** ..... Constant for volume split between underflow and overflow (Default=6.13 if flow rate is in U.S. gallons/min)

EFFICIENCY Use the efficiency table to specify efficiency as a function of particle size. If you do not provide EFFICIENCY, HYCYC uses a built-in correlation to calculate separation efficiency.

- **diam** ..... Diameter of solid particles to be separated
- **eff** ..... Collection efficiency of solid particles to be separated

Accessing Variables in HYCYC

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for an HYCYC block.

Block Input

Sentence	Variables	ID1
SIMULATION	DIAM, NCYCLONE	—
DESIGN	DIAM-PART, EFF, MAX-DIAM, MAX-PDROP, DEN-PART	—
RATIOS	INLET, LENGTH, OVER, UNDER, CONE-ANGLE	—
COEFFICIENTS	VEL-COEF, VEL-EXP, VOL-RATIO	—
EFFICIENCY	DIAM-PARTIC, EFFIC	entryno

Block Results

Description	Sentence	Variable
Calculated diameter	RESULTS	DIAM
Pressure drop	RESULTS	PDROP
Number of hydrocyclones	RESULTS	NCYCLONE
Inlet diameter	RESULTS	DIAM-IN
Length of cylinder	RESULTS	LEN-CYC
Overflow diameter	RESULTS	DIAM-OV
Underflow diameter	RESULTS	DIAM-UN

CFUGE: Centrifuge Filter

Input Language for CFUGE

```
BLOCK    blockid    CFUGE
CENTRIFUGES    diam    revs  /  . . .
CAKE-PROPS    keyword=value
```

Keywords:

CAKE-RES MEDIUM-RES WETNESS

Optional keywords:

POROSITY SPHERICITY DIAM-PART

```
RATIOS    keyword=value
```

Optional keywords:

LIQUID CAKE HEIGHT

Input Language Description for CFUGE

CENTRIFUGES Use to specify diameter and rate of revolution. You must specify both diameter and rate of revolution for at least one centrifuge. If you specify more than one centrifuge, CFUGE selects the smallest suitable one.

diam ..... Diameter

revs ..... Rate of revolution

CAKE-PROPS Use to specify filter cake characteristics. You must specify cake resistance and the resistance of the medium.

CAKE-RES ..... Specific cake resistance. (Use UNITS keyword SPEC-FLT-RESISTANCE to specify units.)

MEDIUM-RES ..... Resistance of the medium. (Use UNITS keyword FILTER-RESISTANCE to specify units.)

WETNESS ..... Moisture content of the filter cake

POROSITY ..... Porosity of the filter cake (Default=0.45)

SPHERICITY ..... Average sphericity of the solid particles in the cake (Default=0.75)

DIAM-PART ..... Average diameter of solid particles in the cake

RATIOS Use to enter optional parameters for ratios of centrifuge dimensions to centrifuge radius.

LIQUID ..... Ratio of the radius of the liquid surface to the radius of the centrifuge (Default=0.738)

CAKE ..... Ratio of the radius of the filter cake surface to the radius of the centrifuge (Default=0.79)

HEIGHT ..... Ratio of the height to the radius of the centrifuge (Default=0.9545)

Accessing Variables in CFUGE

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following table lists variable names and other information needed to sample and/or change variables for a CFUGE block.

Block Input

Sentence	Variables	ID1
CENTRIFUGES	DIAM, REVS	n†
CAKE-PROPS	CAKE-RES, MEDIUM-RES, WETNESS, POROSITY, SPHERICITY, DIAM-PART	—
RATIOS	LIQUID, CAKE, HEIGHT	—

† The DIAM vs. REVS pair specification number. Enter 1 if only one pair is specified.

FILTER: Rotary Vacuum Filter

Input Language for FILTER

BLOCK **blockid** **FILTER**
SIMULATION *keyword=value*

Keywords:

DIAM **WIDTH**

DESIGN *keyword=value*

Keyword:

MAX-PDROP

Optional keyword:

RATIO

OPERATION *keyword=value*

Keyword:

REVS

Optional keyword:

ANGLE

CAKE-PROPS *keyword=value*

Keywords:

SOLID-FRAC **POROSITY** **FILTER-RES** **CAKE-RES** **COMPRES** **DIAM-PART** **SPHERICITY**

MEDIUM-PROPS **MEDIUM-RES=value**

Input Language Description for FILTER

SIMULATION Use to enter parameters for simulation mode calculations. You must specify both the filter diameter and its width. You cannot use SIMULATION if you specified DESIGN.

DIAM ..... Filter diameter

WIDTH ..... Filter width

DESIGN Use to specify parameters for design mode calculations. You must specify the maximum pressure drop. You cannot use DESIGN if you specified SIMULATION.

MAX-PDROP ..... Maximum pressure drop allowed

RATIO ..... Ratio of filter diameter to width (Default=2.0)

OPERATION Use to specify operating conditions and parameters. You must specify the rate of revolution of the filter.

REVS ..... Rate of revolution of the filter

ANGLE ..... Angle of filtration. That is, the angle subtended at the center by the portion of the filter submerged in liquid. (Default=2.0945 radians)

CAKE-PROPS Use to specify optional parameters for the filter cake properties.

SOLID-FRAC ..... Mass fraction of solids in filter cake. (Default is calculated from the average particle diameter, particle sphericity, and cake porosity.)

POROSITY ..... Cake porosity (Default=0.45)

FILTER-RES ..... Specific cake resistance or filtration resistance. (Use UNITS keyword SPEC-FLT-RESISTANCE to specify units.) (Default=$2x10^6$ m/kg)

CAKE-RES ..... Specific cake resistance at unit pressure drop. (Use UNITS keyword SPEC-FLT-RESISTANCE to specify units.)

COMPRES ..... Compressibility factor for cake (Default=0)

DIAM-PART ..... Average diameter of solid particles in filter cake

SPHERICITY ..... Sphericity of particles in filter cake (Default=0.75)

MEDIUM-PROPS ..... Use to specify the resistance of filter medium.

MEDIUM-RES ..... Filter medium resistance. (Use UNITS keyword FILTER-RESISTANCE to specify units.) (Default=0)

Accessing Variables in FILTER

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following table lists variable names and other information needed to sample and/or change variables for a FILTER block.

Block Input

Sentence	Variables
SIMULATION	DIAM, WIDTH
DESIGN	MAX-PDROP, RATIO
OPERATION	REVS, ANGLE
CAKE-PROPS	SOLID-FRAC, POROSITY, FILTER-RES, CAKE-RES, COMPRESS, DIAM-PART, SPHERICITY
MEDIUM-PROPS	MEDIUM-RES

DRYER: Solids Dryer

Input Language for DRYER

```
BLOCK    blockid    DRYER
OPERATION    keyword=value
```

Optional keywords:

PRES HEATIN DEWPTDT

```
EXITMOIST    cid    ssid    [value]    /    cid    ssid    [value]    / ...
SUBS-ATTR    ssid    psdid    value-list
ENTRN-ATTR    ssid    { TOTENTRAIN = value
                      { GEFF – SUBSATT = value - list
```

Input Language Description for DRYER

OPERATION Use to specify operating conditions of dryer. Only one of HEATIN and DEWPTDT can be specified.

PRES	Operating pressure of dryer if positive, or pressure drop if negative. (Default=1 atm)
HEATIN	Heat input in addition to that supplied by inlet streams. (Default=0)
DEWPTDT	Exhaust temperature minus exhaust dew point

EXITMOIST Use to specify exit moisture content of any conventional component(s) in any conventional solid substream (Mass flow of component in substream / total mass flow in substream). The flows of unspecified components in each substream are unchanged. In each solid substream, at least one component with non-zero flow must have an unspecified moisture content.

cid	Conventional component ID
ssid	Conventional solid substream ID
value	Exit moisture content

SUBS-ATTR Use to specify outlet stream values of the particle size distribution for any solid substream modifier by DRYER. Enter one SUBS-ATTR sentence for each substream specified.

ssid	Conventional or non-conventional solid substream ID
psdid	Particle size distribution ID
value-list	List of (mass flow of ssid in particle size increment / total mass flow of ssid) for the PSD increments, over the combined exit streams.

ENTRN-ATTR Use to specify the amount of entrainment of solid particles into the exhaust gas stream (if present). Either an overall value for entrainment or an entrainment curve can be specified.

ssid	Conventional on non-conventional solid substream ID
TOTENTRAIN	Overall entrainment of substream ssid into exhaust (mass flow of ssid in exhaust stream / mass flow of ssid in combined exhaust and product streams) (Default = 0)

GEFF-SUBSATT	Entrainment curve of substream ssid into exhaust (mass flow of ssid in PSD increment in exhaust stream / mass flow of ssid in PSD increment in combined exhaust and product streams) (Default = 0)

Accessing Variables in DRYER

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for a DRYER block.

Block Input

Sentence	Variables	ID1	ID2
PARAM	PRES, MAXIT, TOL	—	—
FLOW/FRAC	FLOW/FRAC	substream ID	stream ID

26 Solids Washers

This chapter describes the input language for models that recover the dissolved components in the entrained liquid of a solids stream, using a washing liquid. The models are:

Model	Description	Purpose	Use
SWASH	Single-stage solids washer	Recovery of dissolved components from an entrained liquid of a solids stream using a washing liquid	Single-stage solids washer
CCD	Countercurrent decanter	Multi-stage recovery of dissolved components from an entrained liquid of a solids stream using a washing liquid	Multi-stage solids washers

SWASH: Single-Stage Solids Washer

Input Language for SWASH

```
BLOCK    blockid    SWASH
PARAM    keyword=value
```

Keywords:

MIX-EFF LS-RATIO PRES

Optional keywords:

TEMP DUTY FLASH-MAXIT FLASH-TOL MAX-ITER CONV-TOL T-EST

Input Language Description for SWASH

PARAM

Use to specify SWASH parameters. You must specify the liquid-to-solids mass ratio in the outlet solids stream.

MIX-EFF	Mixing efficiency of the wash (Default=1)	
LS-RATIO	Liquid-to-solids mass ratio in the outlet solids stream	
PRES	**PRES>0**	Pressure
	PRES≤0	Pressure drop (Default=0)
TEMP	Outlet temperature	
DUTY	Heat duty (Default=0)	
FLASH-MAXIT	Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	
FLASH-TOL	Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	
MAX-ITER	Maximum iterations for energy balance calculations (Default=30)	
CONV-TOL	Tolerance for energy balance calculations (Default=$1x10^{-4}$)	
T-EST	Temperature estimate. Use to aid flash convergence when PRES and DUTY are specified.	

Accessing Variables in SWASH

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for a SWASH block.

Block Input

Sentence	Variables
PARAM	MIX-EFF, LS-RATIO, PRES, TEMP, DUTY, T-EST

Block Results

Description	Sentence	Variable
Heat duty	RESULTS	QCALC
Temperature	RESULTS	TCALC
Net heat duty	RESULTS	NET-DUTY

CCD: Countercurrent Decanter

Input Language for CCD

```
BLOCK    blockid    CCD
PARAM    keyword=value
```

Keywords:

NSTAGE PRES

Optional keywords:

FLASH-MAXIT FLASH-TOL EB-MAXIT EB-TOL TAMB

```
FEEDS    sid    stage    dircode  / ...
PRODUCTS    sid    stage    dircode    [frac]  / ...
T-SPEC    stage    temp  / ...
MIX-EFF    stage    eff  / ...
LS-RATIO    stage    ratio  / ...
HEATERS    stage    keyword=value  / ...
```

Keywords:

DUTY UA TMED

```
T-EST    stage    temp  / ...
PSEUDO-STREAM    sid    stage    dircode    [basis-FLOW]  / ...
```

Input Language Description for CCD

PARAM

Use to specify number of stages and pressure. You can optionally enter ambient temperature and convergence parameters.

NSTAGE..... Number of stages

PRES..... Pressure

FLASH-MAXIT ..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

FLASH-TOL..... Flash convergence tolerance. (Default=value established by SIM-OPTIONS paragraph.) (See Chapter 45.)

EB-MAXIT ..... Maximum iterations for energy balance calculations (Default=30)

EB-TOL..... Tolerance for energy balance calculations (Default=$1x10^{-4}$)

TAMB ..... Ambient temperature (Default=25°C)

FEEDS

Use to enter feed stream stage number and flow direction. A solids stream must enter on *stage1*. A liquid stream must enter on stage NSTAGE.

	sid	Stream ID	
	stage	Stage number	
	dircode	**UNDER**	Feed to underflow entering the stage
		OVER	Feed to overflow entering the stage

PRODUCTS Use to enter outlet stream stage number, flow direction, and fraction withdrawn. A solids stream must leave stage NSTAGE. A liquid stream must leave *stage1*.

sid	Stream ID	
stage	Stage number	
dircode	**UNDER**	Product withdrawn from underflow leaving stage
	OVER	Product withdrawn from overflow leaving stage
frac	Fraction of the stream that is withdrawn (Default=1)	

T-SPEC Use to specify the temperature profile. You cannot use T-SPEC if you specified HEATERS.

stage	Stage number
temp	Temperature

MIX-EFF Use to specify the mixing efficiency profile. You must also specify LS-RATIO.

stage	Stage number
eff	Mixing efficiency

LS-RATIO Use to specify the liquid-to-solid ratio profile. You must also specify MIX-EFF.

stage	Stage number
ratio	Liquid-to-solid mass ratio

HEATERS Use to specify either heat duty or overall heat transfer coefficient. You cannot use HEATERS if you specified T-SPEC.

stage	Stage number
DUTY	Stage heat duty
UA	Overall heat transfer coefficient
TMED	Medium temperature (Default=TAMB)

T-EST Use to specify the estimated stage temperature.

stage	Stage number
temp	Estimated temperature

PSEUDO-STREAM Use to identify the interstage flow as pseudostreams and to enter their locations and flows. If you do not specify a flow rate, the flow of each substream of the interstage will be stored in the pseudoproduct stream.

sid	Stream ID	
stage	Stage number	
dircode	**UNDER**	Interstage underflow
	OVER	Interstage overflow
basis-FLOW	Flow rate on MOLE or MASS basis	

Accessing Variables in CCD

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for a CCD block.

Block Input

Sentence	Variables	ID1
PARAM	NSTAGE, PRES	—
FEEDS	STAGE	sid
PRODUCTS	STAGE	sid
T-SPEC	TEMP	stage
MIX-EFF	MEFF	stage
LS-RATIO	RATIO	stage
HEATERS	DUTY, UA, TMED	stage

Block Results

Description	Sentence	Variable	ID1
Stage heat duty	PROFILE	DUTY	stage
Stage temperature	PROFILE	TEMP	stage

27 Stream Manipulators

This chapter describes the input language for stream manipulators. Use stream manipulators to modify stream variables; they do not represent real unit operations. The models are:

Model	Description	Purpose	Use
MULT	Stream multiplier	Multiply component and total flow rates by a factor	Scaling streams by a factor
DUPL	Stream duplicator	Copy inlet stream into any number of duplicate outlet streams	Duplicating feed or internal streams
CLCHNG	Stream class changer	Change stream class between blocks and flowsheet sections	Adding or deleting empty solid substreams between flowsheet
SELECTOR	Stream selector	Copy the selected input stream to the outlet stream	Selecting a stream from a number of number of inlet streams
QTVEC	Load stream manipulator	Combine heat streams into a load stream, or add a temperature-duty point to a load stream	Creating and adding heat data to load streams
ANALYZER	Stream analyzer	Analyze and report flowsheet stream properties	Reporting stream properties in sequential-modular or offline runs, and analyzing or specifying stream propeties in equation-oriented or online runs

MULT: Stream Multiplier

Input Language for MULT

```
BLOCK    blockid    MULT
PARAM    FACTOR
```

Input Language Description for MULT

PARAM Use to enter the multiplication factor.

FACTOR..... Multiplication factor

Accessing Variables in MULT

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following table lists the variable name needed to sample and/or change variables for a MULT block.

Block Input

Sentence	Variable
PARAM	FACTOR

DUPL: Stream Duplicator

Input Language for DUPL

```
BLOCK    blockid    DUPL
```

CLCHNG: Stream Class Changer

Input Language for CLCHNG

```
BLOCK    blockid    CLCHNG
```

SELECTOR: Stream Selector

Input Language for SELECTOR

```
BLOCK    blockid    SELECTOR
PARAM    STREAM
```

Input Language Description for SELECTOR

PARAM Use to enter the selected inlet stream id.

STREAM ..... Selected inlet stream id

Accessing Variables in SELECTOR

Chapter 29 describes how to access variables. The following table lists the variable name needed to sample and/or change variables for a SELECTOR block. In this case, STREAM is the selected inlet stream sequence number of a Selector block. Therefore, the value for the STREAM variable can range from 1 to N; where N is the number of inlet streams of a selector block.

Block Input

Sentence	Variable
PARAM	STREAM

QTVEC: Load Stream Manipulator

Input Language for QTVEC

```
BLOCK    blockid    QTVEC
PARAM    keyword=value
```

Keywords:

TEMP DELT

Input Language Description for QTVEC

PARAM Use to enter the selected inlet stream id.

TEMP..... Starting temperature of the outlet load stream

DELT ..... Temperature difference between the first two points (TVEC2-TVEC1) of the outlet load stream

ANALYZER: Stream Analyzer

Input Language for ANALYZER

```
BLOCK    blockid    ANALYZER
PARAM    keyword=value
```

Keywords:

STREAM

Optional Keywords:

NPHASE PRES TEMP VFRAC MAXIT TOL

PROPS **propsetid / . . .**
SPC-OPTIONS *keyword=value* **/ . . .**

Keywords:

MOLE-FLOW MASS-FLOW STDVOL-FLOW

Input Language Description for ANALYZER

PARAM Use to enter the stream information and its optional flash specifications.

STREAM	Reference stream ID. Specify STREAM when the Analyzer block is not physically connected to inlet and outlet streams.
NPHASE	Number of phases to be considered in flash calculations. This is defaulted to global Nphase option.
PRES	Flash pressure (Default=stream pressure)
TEMP	Flash temperature. By default this is computed by adiabatic flash.
VFRAC	Flash vapor fraction. By default this is computed by adiabatic flash.
MAXIT	Flash iteration limit. This is defaulted to global flash iteration limit.
TOL	Flash tolerance. This is defaulted to global flash tolerance.

PROPS Use to enter the physical property set ID.

propsetid	Prop-set ID.

SPC-OPTIONS Use to enter options to add additional variables during equation oriented runs.

MOLE-FLOW	**MOLE-FLOW=YES**	Add molar component flows to variable list.
	MOLE-FLOW=NO	Do not add molar component flows to variable list.
MASS-FLOW	**MASS-FLOW=YES**	Add mass component flows to variable list.
	MASS-FLOW=NO	Do not add mass component flows to variable list.
STDVOL-FLOW	**STDVOL-FLOW=YES**	Add standard volume component flows to variable list.
	STDVOL-FLOW=NO	Do not add standard volume component flows to variable list.

Accessing Variables in ANALYZER

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1	ID2	ID3	Element
PARAM	PRES, TEMP, VFRAC, MAXIT, TOL	—	—	—	—

28 User Unit Operation Models

This chapter describes the input language for the user models. The models are:

Model	Description	Purpose	Use
USER	User UOS model	User-supplied model	User-supplied model with up to four material inlet and outlet streams
USER2	User UOS model	User-supplied model	User-supplied model with any number of material inlet and outlet streams
USER3	User UOS model	User-supplied model with SM and EO functionality	User-supplied model with any number of material inlet and outlet streams
ACMMODEL	User UOS model	User-supplied model built in Aspen Custom Modeler	User-supplied model with any number of material inlet and outlet streams
CAPE-OPEN	User UOS model	User-supplied model built to CAPE-OPEN specifications	User-supplied model with any number of material inlet and outlet streams

USER and USER2: User UOS Model

Input Language for USER

```
BLOCK  blockid  USER
SUBROUTINE  model  report
PARAM  keyword=value
```

Keywords:

NINT NREAL NIWORK NWORK NSIZE FLASH-FEEDS BYPASS-USER

```
INT  value-list
REAL  value-list
FLASH-SPECS  sid  kode  keyword=value  /  ...
```

Keywords:

TEMP PRES VFRAC

Optional keywords:

NPHASE PHASE MAXIT TOL FREE-WATER PROPERTIES T-EST P-EST

Input Language for USER2

```
BLOCK  blockid  USER2
SUBROUTINE  model  report
PARAM  keyword=value
```

Keywords:

NINT NREAL NCHAR NIWORK NWORK NSIZE FLASH-FEEDS BYPASS-USER EXCEL-FILE

```
INT  value-list
REAL  value-list
CHAR  char-list
FLASH-SPECS  sid  kode  keyword=value  /  ...
```

Keywords:

TEMP PRES VFRAC

Optional keywords:

NPHASE PHASE MAXIT TOL FREE-WATER PROPERTIES T-EST P-EST

```
USER-MODELS  USER-SUBS="name1" "name2" . . . CONFIG="name"
```

Input Language Description for USER and USER2

USER and USER2 allow you to use user-written unit operation models in an Aspen Plus run. The user model must be in the form of a FORTRAN subroutine, written to specifications described in *Aspen Plus User Models*, Chapter 5. You

can specify up to four material inlet and outlet streams for USER. There are no limitations on the number of inlet or outlet streams for USER2.

blockid ..... User block ID

SUBROUTINE

Use to specify the name of the user-supplied model subroutine. You can also specify the user-supplied report subroutine. For details on writing user-supplied model and report subroutines, see *Aspen Plus User Models*, Chapter 5.

model ..... User-supplied model subroutine name. For USER2 only, this is optional if EXCEL-FILE is specified (see below).

report ..... Optional user-supplied report subroutine name

PARAM

Use to enter flash option and define the length of arrays for user-supplied model and report subroutines.

NINT ..... Length of the integer parameter array (Default=1)

NREAL ..... Length of the real parameter array (Default=1)

NCHAR ..... Length of the character parameter array (Default=1)

NIWORK ..... Length of the integer workspace array (Default=1)

NWORK ..... Length of the real workspace array (Default=1)

NSIZE ..... Length of size array (Default=1)

FLASH-FEEDS ..... Flash all inlet material streams before calling the model subroutine: YES or NO (Default=NO)

BYPASS-USER ..... Bypass the user-supplied model subroutine if the total flow is zero: YES or NO (Default=YES)

EXCEL-FILE ..... Filename for the Excel User Model interface. See *Aspen Plus User Models*, Chapter 5, for more information.

INT

Use to enter values for the integer parameter array of the user model and report subroutines.

value-list ..... List of integer values

REAL

Use to enter values for the real parameter array of the user model and report subroutines.

value-list ..... List of real values

CHAR

Use to enter values for the character parameter array of the user model and report subroutines. See *Aspen Plus User Models*, Chapter 5, for information on how these parameters are used.

char-list ..... List of quoted character values

FLASH-SPECS

Use to specify the thermodynamic conditions for the outlet streams. If you enter *sid*, Aspen Plus will perform a flash calculation at the conditions specified, after the user model FORTRAN subroutine is executed. By default, no flash calculations are performed.

sid ..... Stream ID

kode ..... Thermodynamic condition of flash calculation:

NOFLASH	The outlet stream is not flashed (Default)
PH	PH flash
TP	TP flash
PV	PV flash
TH	TH flash
TV	TV flash

TEMP ..... Temperature. Use when *kode* is TP, TH, or TV.

PRES ..... Pressure. Use when *kode* is PH, TP, or PV.

VFRAC ..... Vapor fraction. Use when *kode* is PV or TV.

NPHASE ..... Number of phases in MIXED substream:

NPHASE=1	One-phase calculation
NPHASE=2	Two-phase flash (Default)
NPHASE=3	Three-phase flash

PHASE ..... Specifies the phase when NPHASE=1:

PHASE=V	Vapor (Default)
PHASE=L	Liquid
PHASE=S	Solid. Use for electrolytes system only.

MAXIT ..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.)
(See Chapter 45.)

TOL ..... Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

FREE-WATER ..... Use to override the free-water option established by the SIM-OPTIONS paragraph. (See Chapter 45.)

FREE-WATER=YES	Performs free-water calculations
FREE-WATER=NO	Does not perform free-water calculations

PROPERTIES ..... Pointer to indicate which property option set specified in the PROPERTIES sentence is to be used. (See Chapter 11.)

PROPERTIES=1	Uses the first property option set listed in the PROPERTIES sentence (Default)
PROPERTIES=2	Uses the second property option set listed in the PROPERTIES sentence

T-EST ..... Temperature estimate. Use to aid flash convergence when *kode* is PH or PV.

P-EST ..... Pressure estimate. Use to aid flash convergence when *kode* is TH or TV.

USER-MODELS See *Aspen Plus User Models*, chapter 5, for information on how to access these subroutines.

USER-SUBS List of names of additional Fortran subroutines called by the User2 model and report subroutines. (Optional)

CONFIG Name of the custom variable definition subroutine used with the Configured Variables sheet in User2, and also the stem of the name of the file. (Optional) See chapter 4 of *Getting Started Customizing Unit Operation Models* for more information about this file.

Accessing Variables in USER and USER2

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following table lists variable names and other information needed to sample and/or change variables for a USER or USER2 block.

Block Input

Sentence	Variables	ID1	Element
FLASH-SPECS	MAXIT, TOL, TEMP, PRES, VFRAC, T-EST, P-EST	sid	—
INT	VALUE-LIST	—	†
REAL	VALUE-LIST	—	†

† Position of a value in the INT or REAL value-list.

USER3: User Dual-Execution Model

Input Language for USER3

```
BLOCK  blockid  USER3
SUBROUTINE  MODEL=subname  [REPORT=subname]  [MODEL1=subname]
PARAM  keyword=value
```

Optional keywords:

MAX-NY MAX-NAE MAX-NZ NINT NREAL AE-METHOD NUMJAC PERSIZ CMPJAC DCRTOL DCATOL MVZERO ZERTOL MVZTOL SUMMARY NCHAR NIWORK NWORK NSIZE FLASH-FEEDS BYPASS-USER

```
MODEL-COMP  COMPS=cgroup
CFG-DIRECTOR  CFG-DIR-WNT="path"
CFG-NAME  CFGNAM=name
SPECS  "vid"  [value]  /  ...
Y  index  INIT=value  STAT=value  MIN=value  MAX=value  SCALE=value / ...
VARIABLES  "vid"  INIT=value  STAT=value  MIN=value  MAX=value  &
     SBND=value  SCALE=value  UNITS='uom'  UNITTYPE=value  /  ...
F  index  STAT=value  SCALE=value  /  ...
FUNCTIONS  "fid"  STAT=value  SCALE=value  /  ...
INT  value-list
INTEGERS  index  value  /  ...
REAL  value-list
CHAR  char-list
FLASH-SPECS  sid  kode  keyword=value  /  ...
```

Keywords:

TEMP PRES VFRAC

Optional keywords:

NPHASE PHASE MAXIT TOL FREE-WATER T-INIT P-INIT

```
USER-MODELS  USER-SUBS="name1" "name2" . . . CONFIG="name"
CONNECT  STREAM=sid  PORT=portid
INTPARAM  NAME=paramid  VALUE=value
REALPARAM  NAME=paramid  VALUE=value  PHYS-QTY=value  UOM=value
STRINGPARAM  NAME=paramid  VALUE=value
```

Input Language Description for USER3

USER3 allows you to use user-written dual-execution unit operation models in an Aspen Plus sequential modular or equation-oriented run. The user model must be in the form of a compiled FORTRAN subroutine written to USER3 specifications. There are no limitations on the number of inlet or outlet streams for USER3. You can also use USER3 with CAPE-OPEN models, but the CAPE-OPEN model type is preferred.

blockid ..... User block ID

SUBROUTINE

Use to specify the name of the user-supplied model subroutine. You can also specify the user-supplied report subroutine.

REPORT..... Optional user-supplied report subroutine name. (Default = same as MODEL subroutine)

MODEL1 ..... Optional additional model subroutine. This is an external routine which the main model subroutine may call.

PARAM

Use to allocate memory space for the model, define the length of arrays for user-supplied model and report subroutines, select a solver, and control the USER3 numeric layer.

MAX-NY ..... Maximum number of model algebraic variables (Default = supplied by model)

MAX-NAE ..... Maximum number of model algebraic equations (Default = supplied by model)

MAX-NZ..... Maximum number of model non-zeroes (Default = supplied by model)

NINT..... Length of the integer parameter array (Default=1)

NREAL..... Length of the real parameter array (Default=1)

AE-METHOD ..... Solver to use for equation-oriented solution

AE-METHOD=DMO	DMO solver (Default)
AE-METHOD=NSOLVE	NSOLVE solver
AE-METHOD=LSSQP	LSSQP solver

NUMJAC ..... Specify whether to use analytic or numeric sparsity pattern and derivatives. Analytic sparsity pattern and derivates are specified by the model subroutine. Use NUMJAC=PARTIAL or FULL to have Aspen Plus compute these numerically.

NUMJAC=NO	Use analytic sparsity pattern and derivatives (Default)
NUMJAC=PARTIAL	Use analytic sparsity pattern and numeric derivatives
NUMJAC=FULL	Use numeric sparsity pattern and derivatives

CMPJAC..... Specify comparisons of analytic and numerical problems to perform. The Jacobians compared must be based on the same sparsity pattern, so CMPJAC=DERIV or ALL cannot be used with NUMJAC=FULL.

CMPJAC=NO	No comparisons (Default)

	CMPJAC=SPAT	Compare sparsity patterns
	CMPJAC=DERIV	Compare derivatives
	CMPJAC=ALL	Compare both sparsity patterns and derivatives

DCRTOL..... Relative tolerance for derivative comparison (default = 10^{-2})

DCATOL..... Absolute tolerance for derivative comparison (default = 10^{-6})

DCRTOL and DCATOL are used during derivative comparisons. If *a* is the value from the analytical Jacobian and *b* is the corresponding value from the numerical Jacobian, then the values are said to be the same when

$$|a-b| \geq DCRTOL \times \max(|a|, DCATOL)$$

PERSIZ..... Numerical perturbation size parameter (default = 10^{-6})

Given a variable with non-scaled value *y* and with scale *s*, the absolute value of the perturbation applied to *y* is: $PERSIZ \times \max(|y|, |s|)$.

MVZERO..... Whether to move zero variable values away from zero before sparsity detection

MVZERO=YES	Move variable values which are zero away from zero before sparsity pattern detection starts (Default)
MVZERO=NO	Leave variable values which are zero at zero

ZERTOL..... Zero tolerance used when MVZERO=YES (default = 10^{-12})

MVZTOL..... Amount to move zero variables when MVZERO=YES (default = 10^{-2})

SUMMARY..... Which data to report. Eliminating some data can speed the loading of a very large model into the Aspen Plus GUI.

SUMMARY=ALL	Report all equations and variables. (Default)
SUMMARY=VARS	Report variables only
SUMMARY=EQNS	Report equations only
SUMMARY=NONE	Report nothing

NCHAR..... Length of the character parameter array (Default=1)

NIWORK..... Length of the integer workspace array (Default=1)

NWORK..... Length of the real workspace array (Default=1)

NSIZE..... Length of size array (Default=1)

FLASH-FEEDS..... Flash all inlet material streams before calling the model subroutine: YES or NO (Default=NO)

BYPASS-USER..... Bypass the user-supplied model subroutine if the total flow is zero: YES or NO (Default=YES)

MODEL-COMP Use to specify a reduced component slate for the block.

COMPS..... Component group ID (defined via the COMP-GROUP primary keyword) defining a reduced component slate for the block. This may not be supported by some USER3 models.

CFG-DIRECTOR Use to specify the directory for the configuration file when using EOPML models.

CFG-DIR-WNT..... Path name of the directory where the configuration file is stored. Must be enclosed in quotes.

CFG-NAME Use to specify the name of the configuration file when using EOPML models.

CFGNAM ..... Name of the EOPML configuration file.

SPECS Use to specify which variables are fixed, and their values. Values entered in the SPECS sentence are passed directly to the model, and not modified in any way. To specify a square problem, you should specify values for *nspec* = *nvariables* – *nequations* variables.

vid ..... Name of the variable to fix. Names are matched from right-to-left and enough of the name must be given to uniquely identify it from other variables. Names must be enclosed in quotation marks.

value..... Value at which the variable is fixed. Providing a value in the SPECS sentence is not required since there are other ways to specify a variable's value (such as via a CALCULATOR block or via the USER3 Y sentence). When a fixed variable does not have a value when a model is executed, the outcome depends on the specific model. Some models might use a default value, other models might report an error and exit.

Y Use to specify the attributes of variables, specifying variables based on their positions in the model variable vector. Values entered in the Y sentence are passed directly to the model, and not modified in any way.

index ..... Variable index (position) in the model variable vector.

INIT..... Variable initial value.

STAT ..... Variable fixed/free status.

STAT=0	Variable is free or calculated (Default)
STAT=1	Variable is fixed

MIN..... Variable lower bound.

MAX ..... Variable upper bound.

SCALE ..... Variable scaling factor.

VARIABLES Use to specify the attributes of variables, specify variables by name.

vid ..... Variable name. Names are matched from right-to-left and enough of the name must be given to uniquely identify it from other variables. Names must be enclosed in quotation marks.

INIT..... Variable initial value.

STAT ..... Variable fixed/free status.

STAT = N	Variable is free or calculated (Default)
STAT = F	Variable is fixed

MIN..... Variable lower bound.

MAX ..... Variable upper bound.

SBND ..... Variable step bound.

SCALE ..... Variable scaling factor.

UNITS ..... Variable units. Must be a valid Aspen Plus units string.

UNITTYPE ..... Numerical code indicating physical type of variable. Commonly used values are 22 for temperature and 31 for temperature change, which are important to distinguish. See the *OOMF Script Language* manual, Chapter 11, for a complete list of these codes.

F Use to specify equation attributes, specifying equations based on their position in the model residual vector.

index ..... Equation index (position) in the model residual vector.

STAT ..... Equation inclusion status.

STAT = 0	Equation is included (Default)
STAT = 1	Equation is not included

SCALE ..... Equation scaling factor.

FUNCTIONS

Use to specify equation attributes, specifying equations by name.

fid ..... Equation name. Names are matched from right-to-left and enough of the name must be given to uniquely identify it from other equations. Names must be enclosed in quotation marks.

STAT ..... Equation inclusion status.

STAT = I	Equation is included (Default)
STAT = N	Equation is not included

SCALE ..... Equation scaling factor.

INT

Use to enter values for the integer parameter array of the user model and report subroutines.

value-list ..... List of integer values. Use * to skip an entry

INTEGERS

Use to enter specific values for the integer parameter array specified by their index in the array.

index ..... Parameter index in the INT array

value..... Integer value

REAL

Use to enter values for the real parameter array of the user model and report subroutines.

value-list ..... List of real values

CHAR

Use to enter values for the character parameter array of the user model and report subroutines. See *Aspen Plus User Models*, Chapter 5, for information on how these parameters are used. When using USER3 with a CAPE-OPEN model, CHAR should contain a single value, the model's class ID.

char-list ..... List of quoted character values

FLASH-SPECS

Use to specify the thermodynamic conditions for the outlet streams. If you enter *sid*, Aspen Plus will perform a flash calculation at the conditions specified, after the user model FORTRAN subroutine is executed. By default, no flash calculations are performed.

sid..... Stream ID

kode..... Thermodynamic condition of flash calculation:

NOFLASH	The outlet stream is not flashed (Default)
PH	PH flash
TP	TP flash
PV	PV flash
TH	TH flash
TV	TV flash

TEMP..... Temperature. Use when *kode* is TP, TH, or TV.

PRES..... Pressure. Use when *kode* is PH, TP, or PV.

VFRAC..... Vapor fraction. Use when *kode* is PV or TV.

NPHASE ..... Number of phases in MIXED substream:

NPHASE=1	One-phase calculation
NPHASE=2	Two-phase flash (Default)

	NPHASE=3	Three-phase flash
PHASE	Specifies the phase when NPHASE=1:	
	PHASE=V	Vapor (Default)
	PHASE=L	Liquid
	PHASE=S	Solid. Use for electrolytes system only.
MAXIT	Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	
TOL	Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)	
FREE-WATER	Use to override the free-water option established by the SIM-OPTIONS paragraph. (See Chapter 45.)	
	FREE-WATER=YES	Performs free-water calculations
	FREE-WATER=NO	Does not perform free-water calculations
T-INIT	Temperature estimate. Use to aid flash convergence when *kode* is PH or PV. TINIT and TEST are alternate forms of this keyword.	
P-INIT	Pressure estimate. Use to aid flash convergence when *kode* is TH or TV. PINIT and PEST are alternate forms of this keyword.	

USER-MODELS

See *Aspen Plus User Models*, chapter 5, for information on how to access these subroutines.

USER-SUBS	List of names of additional Fortran subroutines called by the User3 model and report subroutines. (Optional)
CONFIG	Name of the custom variable definition subroutine used with the Configured Variables sheet, and also the stem of the name of the file. (Optional) See chapter 4 of *Getting Started Customizing Unit Operation Models* for more information about this file.

CONNECT

Use to associate a CAPE-OPEN model port with an Aspen Plus stream.

STREAM	Aspen Plus stream name
PORT	CAPE-OPEN model port name. The port name may need to be enclosed in double quotes.

INTPARAM

Use to enter values for integer CAPE-OPEN parameters.

NAME	Integer parameter name. The parameter name may need to be enclosed in double quotes.
VALUE	Integer parameter value

REALPARAM

Use to enter values for real CAPE-OPEN parameters.

NAME	Real parameter name. The parameter name may need to be enclosed in double quotes.
VALUE	Real parameter value
PHYS-QTY	Real parameter physical quantity type. See Chapter 3.
UOM	Real parameter units of measure. Must be a valid Aspen Plus units of measure string as defined in Chapter 3.

STRINGPARAM

Use to enter values for string CAPE-OPEN parameters.

NAME	String parameter name. The parameter name may need to be enclosed in double quotes.

VALUE..... String parameter value. The parameter name may need to be enclosed in double quotes.

Accessing Variables in USER3

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following table lists variable names and other information needed to sample and/or change variables for a USER3 block.

Block Input

Sentence	Variables	Element
Y	INIT	index†
INT	INT	index†
REAL	RVALUE-LIST	index†

† Position of a value in the Y, INT or REAL value-list.

Block Results

Description	Sentence	Variable	ID1
Variable final values	Y	FINAL	index†

† Position of the variable in the Y value-list.

ACMMODEL: User Unit Operations Model from ACM

Input Language for ACMMODEL

```
BLOCK    blockid    ACMMODEL
PARAM    keyword=value
```

Keywords:

MODEL

Optional Keywords:

USER-BYPASS RES-QUERY AE-METHOD INTER

```
CONNECT    STREAM=sid    PORT=portid
COMPONENT-LIST    CLISTID=value
```

Optional keywords:

COMP-GROUP OPSETNAME HENRY-COMPS CHEMISTRY TRUE-COMPS FREE-WATER SOLU-WATER

```
INTPARAM    NAME=paramid    VALUE=value
REALPARAM   NAME=paramid    VALUE=value   PHYS-QTY=value   UOM=value
STRINGPARAM NAME=paramid    VALUE=value
CLISTPARAM  NAME=paramid    VALUE=value
VARIABLES   vname   VALUE=value   LOWER=value   UPPER=value
      STEP=value   BOUND-TYPE=value   SBWEIGHT=value   PHYS-QTY=value
      UOM=value   SCALE=value   SPEC=value
```

Input Language Description for ACMMODEL

ACMMODEL allows you to use ACM exported unit operation models in an Aspen Plus sequential-modular or equation-oriented run. See ACM documentation for details on how to export models for use with Aspen Plus.

blockid ..... User block ID

PARAM

Use to specify the model name, solver, and whether the model should be bypassed if it has zero inlet flow rate.

MODEL ..... Name of ACM exported model

USER-BYPASS ..... Bypass the ACM block if the total flow is zero: YES or NO (Default=YES)

AE-METHOD ..... Solver to use for the equation-oriented solution.

AEMETHOD = SPARSE	Sparse solver (default)
AEMETHOD = DMO	DMO solver
AEMETHOD = NSOLVE	NSOLVE solver
AEMETHOD = LSSQP	LSSQP solver

RES-QUERY ..... Variable query to execute for model's report.

INTER ..... Interactive run flag: YES or NO (Default=NO)

CONNECT

Use to associate an ACM Model port with an Aspen Plus stream.

STREAM ..... Aspen Plus stream name

PORT ..... ACM Model port name

COMPONENT-LIST

Use to define the component list for the ACM Model. The defined component list can be referenced in the model's component list parameters. A component list consists of a component group and property options.

CLISTID ..... Component list ID

COMP-GROUP ..... Component group ID

OPSETNAME ..... See Specifying Property Options Set in Chapter 8 for details on these keywords.
HENRY-COMPS
CHEMISTRY
TRUE-COMPS
FREE-WATER
SOLU-WATER

INTPARAM

Use to enter values for integer parameters.

NAME ..... Integer parameter name. The parameter name may need to be enclosed in double quotes.

VALUE ..... Integer parameter value

REALPARAM

Use to enter values for real parameters.

NAME ..... Real parameter name. The parameter name may need to be enclosed in double quotes.

VALUE ..... Real parameter value

PHYS-QTY ..... Real parameter physical quantity type. See Chapter 3.

UOM ..... Real parameter units of measure. Must be a valid Aspen Plus units of measure string as defined in Chapter 3.

STRINGPARAM Use to enter values for string parameters.

NAME ..... String parameter name. The parameter name may need to be enclosed in double quotes.

VALUE ..... String parameter value, enclosed in double quotes.

CLISTPARAM Use to enter values for component-list parameters.

NAME ..... Component-list parameter name

VALUE ..... Component-list parameter value

VARIABLES Use to specify the attributes of variables. See Aspen Plus *Getting Started with Equation-Oriented Modeling* or the online help for more information on variable attributes.

vname ..... Variable name. Must be enclosed in quotation marks.

VALUE ..... Variable value

LOWER ..... Variable lower bound

UPPER ..... Variable upper bound

STEP ..... Variable step bound

BOUND ..... Variable bound type

BOUND=HARD	Bound is hard (default)
BOUND=SOFT	Bound is soft
BOUND=RELAXED	Bound is relaxed

SBWEIGHT ..... Variable soft bound weight value

PHYS-QTY ..... Variable physical quantity type. See Chapter 3.

UOM ..... Variable units of measure. Must be a valid Aspen Plus units of measure type. See Chapter 3.

SCALE ..... Variable scaling factor

SPEC ..... Variable specification

SPEC=CALC	Variable is calculated
SPEC=CONST	Variable is fixed
SPEC=INDEP	Variable is independent
SPEC=MEAS	Variable is measured
SPEC=PARAM	Variable is parameterized
SPEC=OPTIM	Variable is optimized
SPEC=RECON	Variable is reconciled
SPEC=INITIAL	Variable value is known and fixed at time zero.

Accessing Variables in ACM Blocks

The variables accessible in ACM blocks depend on the variables configured in the model when it was exported from ACM. See the Aspen Custom Modeler documentation for more details.

CAPE-OPEN: User CAPE-OPEN Unit Operation Model

Input Language for CAPE-OPEN

```
BLOCK    blockid    CAPE-OPEN
PARAM    keyword=value
```

Optional keywords:

NCHAR BYPASS-USER INTER

```
CHAR   "{classid}"
CONNECT    STREAM=sid    PORT=portid
INTPARAM    NAME=paramid    VALUE=value
REALPARAM    NAME=paramid    VALUE=value    PHYS-QTY=value    UOM=value
STRINGPARAM    NAME=paramid    VALUE=value
```

Input Language Description for CAPE-OPEN

CAPE-OPEN allows you to use COM unit operation models implementing the CAPE-OPEN standard in an Aspen Plus sequential modular or equation-oriented run.

blockid ..... User block ID

PARAM Use to specify whether the model should be bypassed if it has zero inlet flow rate.

- **NCHAR** ..... Length of the character parameter array (Should always be 1 for CAPE-OPEN).
- **BYPASS-USER** ..... Bypass the user-supplied model subroutine if the total flow is zero: YES or NO (Default=YES)
- **INTER** ..... Interactive run flag: YES or NO (Default=NO)

CHAR Use to specify the class ID of the CAPE-OPEN model.

- **classid** ..... Class ID of the CAPE-OPEN model to be used. This should be a quoted string of hexadecimal digits in the following format: "{00000000-0000-0000-0000-000000000000}"

CONNECT Use to associate a CAPE-OPEN model port with an Aspen Plus stream.

- **STREAM** ..... Aspen Plus stream name
- **PORT**..... CAPE-OPEN model port name. The port name may need to be enclosed in double quotes.

INTPARAM Use to enter values for integer parameters.

	NAME	Integer parameter name. The parameter name may need to be enclosed in double quotes.
	VALUE	Integer parameter value
REALPARAM	Use to enter values for real parameters.	
	NAME	Real parameter name. The parameter name may need to be enclosed in double quotes.
	VALUE	Real parameter value
	PHYS-QTY	Real parameter physical quantity type. See Chapter 3.
	UOM	Real parameter units of measure. Must be a valid Aspen Plus units of measure string as defined in Chapter 3.
STRINGPARAM	Use to enter values for string parameters.	
	NAME	String parameter name. The parameter name may need to be enclosed in double quotes.
	VALUE	String parameter value, enclosed in double quotes.

Accessing Variables in CAPE-OPEN Models

The variables accessible in CAPE-OPEN models depend on the parameters configured in the model. See *User Models* for details on creating these models.

29 Accessing Flowsheet Variables

This chapter describes the input language used for accessing flowsheet variables for use in DESIGN-SPEC, CALCULATOR, OPTIMIZATION, CONSTRAINT, TRANSFER, SENSITIVITY, CASE-STUDY, DATA-FIT and REPORT-SCALE blocks. The following types of variables are accessible:

- Scalar stream variables.
- Stream and substream vectors.
- Unit operation block variables and vectors.
- Component and substream attribute variables and vectors.
- Chemistry and reaction variables.
- Balance block and pressure relief variables.
- Unary and binary physical property parameters.
- Nonconventional component parameter variables and indirect variables.

The DEFINE, VECTOR-DEF, and VARY sentences of a design specification enable you to sample or manipulate any block or stream variable. CALCULATOR blocks (see Chapter 31), sensitivity blocks (see Chapter 35), REPORT-SCALE (see Chapter 46), constraints and optimization paragraphs (see Chapter 32), and DATA-SET and PROFILE-DATA (see Chapter 38) also use the DEFINE and VECTOR-DEF sentences. Sensitivity blocks (see Chapter 35), case-study blocks (see Chapter 36), optimization paragraphs (see Chapter 32), and regression (see Chapter 38) use the VARY sentence. TRANSFER blocks (Chapter 33) use SET and EQUAL-TO sentences, which are similar to VARY.

Accessed flowsheet variables, with the exception of VECTOR-DEF, are in the units established by the IN-UNITS statement.

Accessing Scalar Stream Variables

Input Language

Stream variables:

```
DEFINE  fvar  STREAM-VAR  STREAM=sid  VARIABLE=svarname
VARY  STREAM-VAR  STREAM=sid  VARIABLE=svarname  &
      [LABEL="line1"  "line2"  "line3"  "line4"]
```

Component flow on a MOLE, MASS, or STDVOL basis:

```
DEFINE  fvar  basis-FLOW  STREAM=sid  COMPONENT=cid
VARY  basis-FLOW  STREAM=sid  COMPONENT=cid  &
      [LABEL="line1"  "line2"  "line3"  "line4"]
```

Component fraction on a MOLE, MASS, or STDVOL basis:

```
DEFINE  fvar  basis-FRAC  STREAM=sid  COMPONENT=cid
```

Stream property:

```
DEFINE  fvar  STREAM-PROP  STREAM=sid  PROPERTY=propsetid
```

Heat stream duty:

```
DEFINE  fvar  INFO-VAR  STREAM=sid  INFO=HEAT  VARIABLE=DUTY
VARY  INFO-VAR  STREAM=sid  INFO=HEAT  VARIABLE=DUTY  &
      [LABEL="line1"  "line2"  "line3"  "line4"]
```

Work stream power:

```
DEFINE  fvar  INFO-VAR  STREAM=sid  INFO=WORK  VARIABLE=POWER
VARY  INFO-VAR  STREAM=sid  INFO=WORK  VARIABLE=POWER  &
      [LABEL="line1"  "line2"  "line3"  "line4"]
```

Input Language Description

fvar..... FORTRAN variable name limited to six characters. Must begin with A-H or O-Z, or be declared double precision. For integer variables, *fvar* must begin with I-N or be declared integer.

sid..... Stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

svarname..... TEMP, PRES, VFRAC, LFRAC, MOLE-FLOW, MASS-FLOW, STDVOL-FLOW, MOLE-ENTHALPY, MASS-ENTHALPY, MOLE-ENTROPY, MASS-ENTROPY, MOLE-DENSITY, or MASS-DENSITY. You cannot use the ENTHALPY, ENTROPY, and DENSITY variables in VARY statements.

line1, line2, line3, line4 ..... A string of up to eight characters enclosed in quotes. The label is used in the report in place of system-generated labels.

cid..... Component ID

propsetid ..... ID of a property set defined by a PROP-SET paragraph consisting of a single scalar property. (See Chapter 41.)

Accessing Stream Vectors

Input Language

```
VECTOR-DEF    farray    STREAM    sid
```

Input Language Description

farray..... FORTRAN array name limited to five characters. Aspen Plus will explicitly declare *farray* as double precision or integer, based on the type of the accessed variable.

sid..... Stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

Accessing Substream Vectors

Input Language

```
VECTOR-DEF    farray    SUBSTREAM    STREAM=sid    SUBSTREAM=ssid
```

Input Language Description

farray..... FORTRAN array name limited to five characters. Must begin with A-H or O-Z, or be declared double precision. For integer variables, *farray* must begin with I-N or be declared integer.

sid..... Stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

ssid..... Substream ID

Accessing Unit Operation Block Variables

Input Language

```
DEFINE   fvar   BLOCK-VAR   BLOCK=blockid   SENTENCE=sentname   &
      VARIABLE=varname   [ID1=id1]   [ID2=id2]   [ID3=id3]   &
      [ELEMENT=element]   [EO-NAME=eovarname]   &
      [DESCRIPTION= description]
VARY   BLOCK-VAR   BLOCK=blockid   SENTENCE=sentname   &
      VARIABLE=varname   [ID1=id1]   [ID2=id2]   [ID3=id3]   &
      [ELEMENT=element]   [LABEL="line1"   "line2"   "line3"   "line4"]
```

Input Language Description

fvar	FORTRAN variable name limited to six characters. Aspen Plus will explicitly declare *fvar* as double precision or integer, based on the type of the accessed variable.
blockid	Block ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.
sentname	Sentence name
varname	Variable name
id1, id2, id3	Variable IDs used to uniquely identify the accessed variable when the variable name alone is not sufficient
element	Position of the accessed variable in the list when the variable name is associated with a list of values
eovarname	Equation-Oriented variable name which is equivalent to the accessed variable. A string of up to 32 characters enclosed in quotes.
description	A descriptive string of up to 16 characters enclosed in quotes.
line1, line2, line3, line4	A string of up to eight characters enclosed in quotes. The label is used in the report in place of system-generated labels.

The variables that can be accessed are shown in the Accessing Variables sections in Chapters 12 through 28.

Accessing Unit Operation Block Vectors

Input Language

```
VECTOR-DEF   farray   PROFILE   BLOCK=blockid   SENTENCE=sentname   &
      VARIABLE=varname   [EO-NAME=eovarname]   [DESCRIPTION=description]
```

Input Language Description

farray..... FORTRAN array name limited to five characters. Aspen Plus will explicitly declare *farray* as double precision or integer, based on the type of the accessed variable.

blockid..... Block ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

sentname..... Sentence name

varname ..... Variable name

eovarname..... Equation-Oriented variable name which is equivalent to the accessed variable. A string of up to 32 characters enclosed in quotes.

description..... A descriptive string of up to 16 characters enclosed in quotes

The profile is stored in a FORTRAN array named *farray*. The total length of the array is stored in a second FORTRAN variable, *Lfarray*.

The column profile results that can be accessed are shown in the Accessing Variables sections in Chapters 12 through 28.

Accessing Component Attribute Variables

Input Language

```
DEFINE  fvar  COMP-ATTR-VAR  STREAM=sid  SUBSTREAM=ssid  &
        COMPONENT=cid  ATTRIBUTE=cattrname  [ELEMENT=element]
VARY  COMP-ATTR-VAR  STREAM=sid  SUBSTREAM=ssid  &
        COMPONENT=cid  ATTRIBUTE=cattrname  [ELEMENT=element]  &
        [LABEL="line1"  "line2"  "line3"  "line4"]
```

Input Language Description

fvar..... FORTRAN variable name limited to six characters. Aspen Plus will explicitly declare *fvar* as double precision or integer, based on the type of the accessed variable.

sid..... Stream ID

ssid..... Substream ID

cid..... Component ID

cattrname..... Component attribute name

element ..... Position of the accessed variable in the list when the component attribute name is associated with a list of values

line1, line2, line3, line4..... A string of up to eight characters enclosed in quotes. The label is used in the report in place of system-generated labels.

Accessing Component Attribute Vectors

Input Language

```
VECTOR-DEF  farray  COMP-ATTR  STREAM=sid  SUBSTREAM=ssid  &
      COMPONENT=cid  ATTRIBUTE=cattrname
```

Input Language Description

farray ..... FORTRAN array name limited to five characters. Aspen Plus will explicitly declare *fvar* as double precision or integer, based on the type of the accessed variable.

sid ..... Stream ID

ssid ..... Substream ID

cid ..... Component ID

cattrname ..... Component attribute name

Accessing Substream Attribute Variables

Input Language

```
DEFINE  fvar  SUBS-ATTR-VAR  STREAM=sid  SUBSTREAM=ssid  &
      ATTRIBUTE=sattrname  [ELEMENT=element]
VARY  SUBS-ATTR-VAR  STREAM=sid  SUBSTREAM=ssid  &
      ATTRIBUTE=sattrname  [ELEMENT=element]  &
      [LABEL="line1"  "line2"  "line3"  "line4"]
```

Input Language Description

fvar ..... FORTRAN variable name limited to six characters. Must begin with A-H or O-Z, or be declared double precision. For integer variables, *fvar* must begin with I-N or be declared integer.

sid ..... Stream ID

ssid ..... Substream ID

sattrname ..... Substream attribute name

element ..... Position of the accessed variable in the list when the substream attribute name is associated with a list of values

line1, line2, line3, line4 ..... A string of up to eight characters enclosed in quotes. The label is used in the report in place of system-generated labels.

Accessing Substream Attribute Vectors

Input Language

```
VECTOR-DEF  farray  SUBS-ATTR  STREAM=sid  SUBSTREAM=ssid  &
      ATTRIBUTE=sattrname
```

Input Language Description

farray ..... FORTRAN array name limited to five characters. Aspen Plus will explicitly declare *farray* as double precision or integer, based on the type of the accessed variable.

sid ..... Stream ID

ssid ..... Substream ID

sattrname ..... Substream attribute name

Accessing Chemistry and Reaction Variables

Input Language

Chemistry variables:

```
DEFINE  fvar  CHEM-VAR  CHEMISTRY=chemid  SENTENCE=sentname  &
      VARIABLE=varname  [ID1=id1]  [ID2=id2]
VARY  CHEM-VAR  CHEMISTRY=chemid  SENTENCE=sentname  &
      VARIABLE=varname  [ID1=id1]  [ID2=id2]  &
      [LABEL="line1"  "line2"  "line3"  "line4"]
```

Reaction variables:

```
DEFINE  fvar  REACT-VAR  REACTION=reacid  SENTENCE=sentname  &
      VARIABLE=varname  [ID1=id1]  [ID2=id2]
VARY  REACT-VAR  REACTION=reacid  SENTENCE=sentname  &
      VARIABLE=varname  [ID1=id1]  [ID2=id2]  &
      [LABEL="line1"  "line2"  "line3"  "line4"]
```

Input Language Description

fvar ..... FORTRAN variable name limited to six characters. Aspen Plus will explicitly declare *fvar* as double precision or integer, based on the type of the accessed variable.

chemid ..... Chemistry ID. (See Chapter 5.)

reacid ..... Reaction ID. (See Chapter 6.)

sentname..... Sentence name. (See Accessing Variables sections in Chapters 5 and 6.)

varname ..... Variable name. (See Accessing Variables sections in Chapters 5 and 6.)

id1, id2 ..... Variable IDs used to uniquely identify the accessed variable when the variable name alone is not sufficient.
(See Accessing Variables sections in Chapters 5 and 6.)

line1, line2, line3, line4..... A string of up to eight characters enclosed in quotes. The label is used in the report in place of system-generated labels.

Accessing Balance Block Variables

Input Language

```
DEFINE fvar BALANCE-VAR BLOCK=balanceid SENTENCE=sentname &
      VARIABLE=varname [ID1=id1] [ID2=id2] [EO-NAME=eovarname] &
      [DESCRIPTION=description]
VARY BALANCE-VAR BLOCK=balanceid SENTENCE=sentname &
      VARIABLE=varname [ID1=id1] [ID2=id2] [LABEL="line1" "line2" &
      "line3" "line4"]
```

Input Language Description

fvar..... FORTRAN variable name limited to six characters. Aspen Plus will explicitly declare *fvar* as double precision or integer, based on the type of the accessed variable.

balanceid ..... Block ID

sentname..... Sentence name. (See Accessing Variable section in Chapter 34.)

varname ..... Variable name. (See Accessing Variable section in Chapter 34.)

id1, id2 ..... Variable IDs used to uniquely identify the accessed variable when the variable name alone is not sufficient.
(See Accessing Variable section in Chapter 34.)

eovarname..... Equation-Oriented variable name which is equivalent to the accessed variable. A string of up to 32 characters enclosed in quotes.

description..... A descriptive string of up to 16 characters enclosed in quotes

line1, line2, line3, line4..... A string of up to eight characters enclosed in quotes. The label is used in the report in place of system-generated labels.

Accessing Pressure Relief Block Variables

Input Language

```
DEFINE  fvar  PRESR-VAR  BLOCK=pblockid  SENTENCE=sentname  &
      VARIABLE=varname  [ID1=id1]  [EO-NAME=eovarname] &
      [DESCRIPTION=description]
VARY  PRESR-VAR  BLOCK=pblockid  SENTENCE=sentname  &
      VARIABLE=varname  [ID1=id1]  [LABEL="line1"  "line2"  "line3"  "line4"]
```

Input Language Description

fvar ..... FORTRAN variable name limited to six characters. Aspen Plus will explicitly declare *fvar* as double precision or integer, based on the type of the accessed variable.

pblockid ..... Pressure relief block ID

sentname ..... Sentence name. (See Accessing Variable section in Chapter 39.)

varname ..... Variable name. (See Accessing Variable section in Chapter 39.)

id1 ..... Variable IDs used to uniquely identify the accessed variable when the variable name alone is not sufficient. (See Accessing Variable section in Chapter 39.)

eovarname ..... Equation-Oriented variable name which is equivalent to the accessed variable. A string of up to 32 characters enclosed in quotes.

description ..... A descriptive string of up to 16 characters enclosed in quotes.

line1, line2, line3, line4 ..... A string of up to eight characters enclosed in quotes. The label is used in the report in place of system-generated labels.

Accessing Unary Physical Property Parameters

Input Language

Unary parameter variables:

```
DEFINE  fvar  UNARY-PARAM  VARIABLE=upvarname  [ID1=id1]  [ID2=id2]
VARY  UNARY-PARAM  VARIABLE=upvarname  [ID1=id1]  [ID2=id2]  &
      [LABEL="line1"  "line2"  "line3"  "line4"]
```

Unary correlation element variables:

```
DEFINE  fvar  UNARY-COR-EL  VARIABLE=ucvarname  [ID1=id1]  [ID2=id2]
      & [ELEMENT=element]
VARY  UNARY-COR-EL  VARIABLE=ucvarname  [ID1=id1]  [ID2=id2]  &
      [ELEMENT=element]  [LABEL="line1"  "line2"  "line3"  "line4"]
```

Unary correlation vectors:

```
DEFINE  fvar  UN-COR-VEC  VARIABLE=ucvarname  [ID1=id1]  [ID2=id2]
```

Input Language Description

fvar ..... FORTRAN variable name limited to six characters. Aspen Plus will explicitly declare *fvar* as double precision or integer, based on the type of the accessed variable.

upvarname ..... Scalar unary parameter name, for example OMEGA for Pitzer acentric factor. (See *Aspen Plus Physical Property Methods and Models*, Chapter 3.)

ucvarname ..... Unary correlation parameter name, for example PLXANT for extended Antoine vapor pressure parameter. (See *Aspen Plus Physical Property Methods and Models*, Chapter 3.)

id1, id2 ..... Variable IDs used to uniquely identify the accessed variable when the variable name alone is not sufficient. *id1* is the component ID. *id2* is the parameter data set number. (Default=1)

element ..... Element number of the correlation parameter

line1, line2, line3, line4 ..... A string of up to eight characters enclosed in quotes. The label is used in the report in place of system-generated labels.

Accessing Binary Physical Properties

Input Language

Binary parameter variables:

```
DEFINE  fvar  BI-PARAM  VARIABLE=bpvarname  [ID1=id1]  [ID2=id2]  &
      [ID3=id3]
VARY  UNARY-PARAM  VARIABLE=bpvarname  [ID1=id1]  [ID2=id2]
      [ID3=id3] & [LABEL="line1"  "line2"  "line3"  "line4"]
```

Binary correlation element variables:

```
DEFINE  fvar  BI-COR-EL  VARIABLE=bcvarname  [ID1=id1]  [ID2=id2]  &
      [ID3=id3]  [ELEMENT=element]
VARY  BI-COR-EL  VARIABLE=bcvarname  [ID1=id1]  [ID2=id2]  [ID3=id3]
      &  [ELEMENT=element]  [LABEL="line1"  "line2"  "line3"  "line4"]
```

Binary correlation vectors:

```
DEFINE  fvar  BI-COR-VEC  VARIABLE=bcvarname  [ID1=id1]  [ID2=id2]  &
      [ID3=id3]
```

Input Language Description

fvar ..... FORTRAN variable name limited to six characters. Aspen Plus will explicitly declare *fvar* as double precision or integer, based on the type of the accessed variable.

bpvarname ..... Scalar binary parameter name, for example PRKIJ for the Peng-Robinson equation-of-state model. (See *Aspen Plus Physical Property Methods and Models*, Chapter 3.)

bcvarname ..... Binary correlation parameter name, for example HENRY for Henry's constants. (See *Aspen Plus Physical Property Methods and Models*, Chapter 3.)

id1, id2, id3 ..... Variable IDs used to uniquely identify the accessed variable when the variable name alone is not sufficient. *id1* is the component ID of the first component. *id2* is the component ID of the second component. *id3* is the parameter data set number. (Default=1)

element ..... Element number of the correlation parameter

line1, line2, line3, line4 ..... A string of up to eight characters enclosed in quotes. The label is used in the report in place of system-generated labels.

Accessing Non-Conventional Component Parameter Variables

Input Language

```
DEFINE fvar NC-PARAM VARIABLE=varname [ID1=id1] [ID2=id2] &
      [ELEMENT=element]
VARY NC-PARAM VARIABLE=varname [ID1=id1] [ID2=id2] &
      [ELEMENT=element]
```

Input Language Description

fvar ..... FORTRAN variable name limited to six characters. Aspen Plus will explicitly declare *fvar* as double precision or integer, based on the type of the accessed variable.

varname ..... Nonconventional component parameter variable name, for example BOIEC parameter for the Boie heat of combustion correlation for coal. (See *Aspen Plus Physical Property Methods and Models*, Chapter 3.)

id1, id2 ..... Variable IDs used to uniquely identify the accessed variable when the variable name alone is not sufficient. *id1* is the component ID of the nonconventional component. *id2* is the data set number which should be set to 1.

element ..... Element number of the vector parameter

Accessing Indirect Variables

Input Language

```
DEFINE  fvar  PARAMETER  paramno  [EO-NAME=eovarname] &
        [INIT-VAL=initval]  [PHYS-QTY=physqty]  [UOM=uom] &
        [DESCRIPTION=description]
VARY  PARAMETER  paramno  [LABEL="line1"  "line2"  "line3"  "line4"]
```

Input Language Description

The PARAMETER variable type is used for direct communication between DEFINE and VARY sentences in different paragraphs. PARAMETER variables are established by the user and create intermediate storage locations used to manipulate, store and retrieve variables that are not direct Aspen Plus block and stream variables, such as the temperature difference between two blocks or the set point of a design specification. PARAMETER variables are identified by the PARAMETER variable number. There can be any number of PARAMETER variables in a simulation.

fvar	FORTRAN variable name limited to six characters. Aspen Plus will explicitly declare *fvar* as double precision or integer, based on the type of the accessed variable.
paramno	Parameter variable number
eovarname	A string of up to eight characters enclosed in quotes. The label is used in the report in place of system-generated labels.
initval	Initial value of the parameter.
physqty	Physical quantity (see Chapter 3) for the accessed variable.
uom	Unit of measure (See Chapter 3).
description	A descriptive string of up to 16 characters in quotes.
line1, line2, line3, line4	A string of up to eight characters enclosed in quotes. The label is used in the report in place of system-generated labels.

30 Design Specifications

This chapter describes the input language for defining design specifications.

Use the DESIGN-SPEC paragraph to:

- Identify the sampled flowsheet variables and equivalence them to FORTRAN variables, by using the DEFINE or VECTOR-DEF sentences.
- Identify a flowsheet variable as the manipulated variable by using the VARY sentence.
- Supply a tolerance on the design specification by using the TOL-SPEC sentence.
- Supply upper and lower limits, and initial and maximum step sizes, for the manipulated variable, using the LIMITS sentence.
- Enter the design specification as a function of the FORTRAN variables, by using the SPEC sentence and optional inline FORTRAN statements.

Accessed flowsheet variables, with the exception of VECTOR-DEF, are in units established by the IN-UNITS statement. You cannot specify alternative units through the use of brackets or braces. A DESIGN-SPEC can only access flowsheet objects which are global (such as property parameters) or which are contained (directly or indirectly) in the hierarchy where the DESIGN-SPEC is specified.

DESIGN-SPEC Paragraph

Input Language for DESIGN-SPEC

```
DESIGN-SPEC    specid
F              FORTRAN declaration statements
DEFINE    fvar    vartype    keyword=value
VECTOR-DEF    farray    vectype    keyword=value
F              Executable FORTRAN statements
SPEC    "expression1"    TO    "expression2"
TOL-SPEC    "tol"
VARY    vartype    keyword=value
LIMITS    "lower"    "upper"    keyword=value
```

Optional keywords for LIMITS:

STEP-SIZE MAX-STEP-SIZE

```
EO-OPTIONS  keyword=value
```

Optional keywords:

COMPS DERIV-METHOD SOLVE-METHOD

```
INIT-ATTR  vname  keyword=value
```

Optional keywords:

VALUE LOWER UPPER STEP BOUND-TYPE SBWEIGHT PHYS-QTY UOM SCALE

```
SCRIPTS  keyword=value
```

Optional keywords:

METHOD TYPE LOCALSCRIPT GLOBALSCRIPT FILE

Input Language Description for DESIGN-SPEC

specid ..... Design specification ID

FORTRAN Statements

Use in computing the design specification function and tolerance, and the manipulated variables limits. FORTRAN statements are needed only if the functions involved are too complex to be represented by the SPEC, TOL-SPEC, and LIMITS expressions. You can also use FORTRAN comments (not shown). See Chapter 31 and the *Aspen Plus User Guide* for a complete discussion of FORTRAN statements and expressions.

DEFINE

Use to access a sampled flowsheet variable and equivalence it to the FORTRAN variable *fvar*, which is used in subsequent FORTRAN statements or expressions to represent the flowsheet variable. There must be at least one DEFINE or VECTOR-DEF sentence in a design specification. Sampled variables are in the input units in effect for the design specification. Stream variables, stream properties, block input variables, and block results can be sampled.

fvar ..... FORTRAN variable name limited to six characters. Aspen Plus will explicitly declare *fvar* as double precision or integer, based on the type of the accessed variable.

vartype ..... Sampled variable type:

BLOCK-VAR	Unit operation block variable

PARAMETER	User-defined indirect variable
STREAM-VAR	Stream variable
basis-FLOW	Component flow on a MOLE, MASS, or STDVOL basis
basis-FRAC	Component fraction on a MOLE, MASS, or STDVOL basis
STREAM-PROP	Stream property, defined using a PROP-SET paragraph. (See Chapter 41.)
INFO-VAR	Heat stream duty or work stream power
COMP-ATTR-VAR	Component attribute variable
SUBS-ATTR-VAR	Substream attribute variable
CHEM-VAR	Chemistry variable
REACT-VAR	Reaction variable
BALANCE-VAR	Balance block variable
PRES-VAR	Pressure relief variable
UNARY-PARAM	Unary parameter variable
UNARY-COR-EL	Unary correlation variable
UN-COR-VEC	Unary correlation vector
BI-PARAM	Binary parameter variable
BI-COR-EL	Binary correlation variable
BI-COR-VEC	Binary correlation vector
NC-PARAM	Non-conventional component parameter variable

The remaining keywords for DEFINE depend on *vartype*. (See Chapter 29.)

VECTOR-DEF Similar to DEFINE except that VECTOR-DEF equivalences an entire stream or block profile result to the FORTRAN array, *farray*. VECTOR-DEF is useful when several variables from the same array are needed. There must be at least one DEFINE or VECTOR-DEF sentence in a design specification.

farray..... FORTRAN array name limited to five characters. Aspen Plus will explicitly declare *farray* as double precision or integer, based on the type of the accessed variable.

vectype..... Sampled vector type:

STREAM	Stream vector
SUBSTREAM	Substream vector
PROFILE	Block vector
COMP-ATTR	Component attribute vector
SUBS-ATTR	Substream attribute vector

The remaining keywords for VECTOR-DEF depend on *vectype*. (See Chapter 29.)

SPEC Use to define the design specification function: *expression1* – *expression2* = 0

Where *expression1* and *expression2* are any valid FORTRAN arithmetic expressions. Typically, *expression1* is a sampled flowsheet variable, and *expression2* is a desired value for the variable, in which case you can omit the quotes ("). You must enter the SPEC sentence.

TOL-SPEC Use to enter the design specification tolerance. $-tol < expression1 - expression2 < tol$

Where *tol* is any valid FORTRAN arithmetic expression. Typically, *tol* is a constant, in which case you can omit the quotes ("). You must enter the TOL-SPEC sentence. Tolerance values specified in the DESIGN-SPEC paragraph are superseded by tolerance values specified in a CONVERGENCE paragraph.

VARY

Use to identify the manipulated variable. You can only manipulate block input or process feed stream variables. You cannot manipulate integer block input variables (for example, the feed location of a distillation column). The manipulated block or stream variable must either be a variable that you specify in the BLOCK or STREAM paragraph, or it must have a default value. The specified or default value is used as an initial estimate by the design specification. The initial guess used for a manipulated variable is the stream or block input specification for the variable. You must enter the VARY sentence. See Chapter 29 for a complete discussion of the VARY sentence. The remaining keywords for VARY depend on *vartype*. (See Chapter 29.)

LIMITS

Use to specify limits for the manipulated variable, where *lower* and *upper* are any valid FORTRAN arithmetic expressions. LIMITS expressions are evaluated before the first iteration of design specification convergence loops. They are not re-evaluated before subsequent iterations. Typically the limits are constants, in which case you can omit the quotes ("). You must enter the LIMITS sentence. You can also use the LIMITS sentence to enter initial step size and maximum step size:

STEP-SIZE..... Initial step size for the manipulated variable. Step size is defined as a fraction of the range (upper limit minus lower limit). Values entered in a CONVERGENCE paragraph supersede values entered in the DESIGN-SPEC paragraph.

MAX-STEP-SIZE ..... Maximum step size for the manipulated variable. Step size is defined as a fraction of the range (upper limit minus lower limit). Values entered in a CONVERGENCE paragraph supersede values entered in the DESIGN-SPEC paragraph.

EO-OPTIONS

Use to specify equation-oriented options for the Design Spec.

COMPS ..... Component group for a list of components which can be active in this Design Spec.

DERIV-METHOD ..... Preferred derivatives method, Analytic or Numeric. Update methods should not be used for Degree of Freedom run modes (Optimization or Reconciliation).

DERIV-METHOD = ANALYTICAL	Model derivatives (Jacobian) are determined from coded analytic expressions. Generally the preferred method.
DERIV-METHOD = NUMERICAL	Alternate method for calculating Jacobian. Useful when there is concern that analytic derivatives are causing convergence difficulties. Usually slower than analytic derivatives, more subject to precision issues. (Default)
DERIV-METHOD = UPDATE-ANALY	Use Schubert method for updating Jacobian, with analytic derivatives for the Base Jacobian. Use when Jacobian calculation is rate limiting step. May result in more iterations and be less robust than calculated derivatives.
DERIV-METHOD = UPDATE-NUMER	Use Schubert method for updating Jacobian, with numerical derivatives for the Base Jacobian. Use when Jacobian calculation is rate limiting step. May result in more iterations and be less robust than calculated derivatives.

SOLVE-METHOD ..... EO solution method. Specifies if open, closed, or neither method should be used with desired action and message level on failure.

SOLVE-METHOD= DO-NOT-CREAT	Ignore during EO solution. (Default)
SOLVE-METHOD= PERTURBATION	Closed solution method; use Perturbation layer around closed model.

INIT-ATTR Use to specify the attributes of open variables.

vname ..... Name of the variable. (Required)

VALUE ..... Current value of the variable.

LOWER ..... Lower bound.

UPPER ..... Upper bound.

STEP ..... Step bound.

BOUND-TYPE ..... Bound type.

BOUND-TYPE = HARD	Do not violate the upper and/or lower bounds when solving a non-square (optimization or data regression) problem.
BOUND-TYPE = RELAXED	Relax upper and/or lower bound. If the initial value is outside the bound, set the bound to the initial value.
BOUND-TYPE = SOFT	Same as relaxed but add a penalty term to the objective to try to drive the value back to the bound.

SBWEIGHT ..... Soft bound weight.

PHYS-QTY ..... The physical quantity that the variable represents, for example, mole flow, temperature, or pressure. These types correspond to the standard Aspen Plus types.

UOM ..... Units of measure (standard Aspen Plus units), based on the physical type of the variable. Internally, all values are stored in SI units.

SCALE ..... Scale factor used by the solver.

SCRIPTS Use this sentence to specify scripts for a block.

METHOD ..... Script method. Blocks support default script methods of SETUP and INIT. User may define other methods. (Required)

TYPE ..... Type of script (Required)

TYPE = LOCALSCRIPT	Local Script
TYPE = GLOBALSCRIPT	Global Script
TYPE = FILE	File

LOCALSCRIPT ..... ID of a LOCAL SCRIPT paragraph. See Chapter 48.

GLOBALSCRIPT ..... ID of a GLOBAL SCRIPT paragraph. See Chapter 48.

FILE ..... Name of a file

31 Calculator Blocks

This chapter describes the input language for CALCULATOR blocks.

Use the CALCULATOR block paragraph to:

- Access the flowsheet variables that are used in the FORTRAN statements and equivalence them to FORTRAN variables, using DEFINE and VECTOR-DEF sentences.
- Supply the FORTRAN statements.
- Designate when the statements are to be executed, by using the EXECUTE sentence, the READ-VARS and WRITE-VARS sentences, or the SEQUENCE paragraph. (See Chapter 37.).
- Specify tear variables to be converged.

CALCULATOR blocks can also be used to manipulate flowsheet variables in EXCEL spreadsheets. This feature can only be used when the CALCULATOR is executed from within the Aspen Plus User Interface.

Accessed flowsheet variables, with the exception of VECTOR-DEF, are in units established by the IN-UNITS statement. You cannot specify alternative units through the use of brackets or braces.

Calculator Block Paragraph

Input Language for CALCULATOR

CALCULATOR cblockid
F *FORTRAN declaration statements*
DEFINE fvar vartype *keyword=value*
VECTOR-DEF farray vectype *keyword=value*
F *Executable FORTRAN statements*
READ-VARS fvar-list
WRITE-VARS fvar-list
EXECUTE executionopt blocktype blockid

Executionopts:

FIRST LAST BEFORE AFTER REPORT

Blocktypes:

BLOCK CONVERGENCE TRANSFER CALCULATOR BALANCE PRES-RELIEF

TEAR-VARS *keyword=value*

Keywords:

TEAR-VAR LOWER UPPER SCALE STEP MAX-STEP

FLASH-SPECS sid kode *keyword=value*

Keywords:

TEMP PRES VFRAC

Optional keywords:

NPHASE PHASE FREE-WATER MAXIT TOL T-EST P-EST

BLOCK-OPTIONS *keyword=value*

Keywords:

SIM-LEVEL TERM-LEVEL VAR-LEVEL TVAR-LEVEL

EO-OPTIONS keyword=value

Optional keywords:

COMPS DERIV-METHOD SOLVE-METHOD

INIT-ATTR *vname* keyword=value

Optional keywords:

VALUE LOWER UPPER STEP BOUND-TYPE SBWEIGHT PHYS-QTY UOM SCALE

SCRIPTS keyword=value

Optional keywords:

METHOD TYPE LOCALSCRIPT GLOBALSCRIPT FILE

cblockid ..... CALCULATOR block ID

DEFINE, VECTOR-DEF

Use to access a flowsheet variable and equivalence it to the FORTRAN variable *fvar*, which is used in subsequent FORTRAN statements to represent the flowsheet variable. VECTOR-DEF is similar to DEFINE, except that VECTOR-DEF equivalences an entire stream or block profile result to the FORTRAN array, *farray*. VECTOR-DEF is useful when several variables from the same array are needed or changed. There must be at least one DEFINE or VECTOR-DEF sentence in a CALCULATOR block. See Chapter 29 for a complete description of the DEFINE and VECTOR-DEF sentences.

FORTRAN Statements

A FORTRAN statement is any valid FORTRAN statement subject to the restrictions discussed in the *Aspen Plus User Guide*. You can also use FORTRAN comments (not shown). Variables accessed using STREAM-PROP, MOLE-FRAC, MASS-FRAC, or STDVOL-FRAC cannot be changed by FORTRAN statements. However, you can use MOLE-FLOW, MASS-FLOW, and STDVOL-FLOW to change stream composition.

READ-VARS, WRITE-VARS

Use to establish which of the variables appearing in DEFINE or VECTOR-DEF sentences are sampled variables, and which are variables changed by the CALCULATOR block. Aspen Plus uses this information to automatically sequence the CALCULATOR block. READ-VARS establishes information flow from the block or stream containing a sampled (read-only) variable to the CALCULATOR block. WRITE-VARS establishes information flow from the CALCULATOR block to changed (read-write or write-only) variables. Do not use the READ-VARS and WRITE-VARS sentences if you specified the EXECUTE sentence.

fvar-list..... List of FORTRAN variables

EXECUTE

Use to specify when the FORTRAN statements are executed. A CALCULATOR block can have only one EXECUTE sentence. If the CALCULATOR block ID is entered in a user-supplied sequence, the EXECUTE sentence is not required. Do not use the EXECUTE sentence if you specified READ-VARS and WRITE-VARS sentences.

executionopt..... Execution options:

FIRST	CALCULATOR block executed at beginning of simulation
LAST	CALCULATOR block executed at end of simulation
BEFORE	CALCULATOR block executed before a block, specified by *blocktype* and *blockid*
AFTER	CALCULATOR block executed after a block, specified by *blocktype* and *blockid*
REPORT	CALCULATOR block executed while report is being generated

blocktype..... Block types. Use only for BEFORE and AFTER execution options.

BLOCK	Unit operation block
CONVERGENCE	Convergence block
TRANSFER	Transfer block
CALCULATOR	CALCULATOR block
BALANCE	Balance block
PRES-RELIEF	Pressure relief block

blockid..... Block ID of the specified *blocktype*. Use only for BEFORE and AFTER execution options.

TEAR-VARS

Use to specify tear variables to be converged.

TEAR-VAR ..... FORTRAN name from WRITE-VARS sentence

LOWER..... Lower limit for the TEAR-VAR for convergence methods that use bounds (Default=-1×10^{35})

UPPER..... Upper limit for the TEAR-VAR for convergence methods that use bounds (Default=$1x10^{35}$)

SCALE ..... Magnitude of the TEAR-VAR to scale the variable with

STEP ..... Relative perturbation step for convergence methods that require perturbation

MAX-STEP ..... Relative step limit per iteration for convergence methods that use the information

FLASH-SPECS

Use to specify the thermodynamic condition of a stream accessed by a CALCULATOR block. Or use to request or suppress flash calculations.

If you do not use FLASH-SPECS, Aspen Plus decides whether or not to flash the stream. Aspen Plus:

- Does not flash a stream if all its variables are declared as READ-VARS only
- Does not flash a stream if the only accessed variables are total flow, enthalpy, entropy, or density
- Flashes a stream if any of the stream variables are declared as WRITE-VARS
- Flashes a stream if the temperature, pressure, or composition of the stream is modified

If Aspen Plus determines that a flash is necessary, it uses the values present in the stream, and the flash options established in the STREAM paragraph or source block of the stream.

sid..... Stream ID

kode..... Thermodynamic condition of flash calculation:

NOFLASH	Stream is not flashed
PH	PH flash
TP	TP flash
PV	PV flash
TH	TH flash
TV	TV flash

TEMP..... Temperature. Allowed only when *kode* is TP, TH, or TV. (Default=value present in the stream)

PRES..... Pressure. Allowed only when *kode* is PH, TP, or PV. (Default=value present in the stream)

VFRAC..... Vapor fraction. Allowed only when *kode* is PV or TV. (Default=value present in the stream)

NPHASE ..... Number of phases in MIXED substream:

NPHASE=1	One-phase calculation
NPHASE=2	Two-phase flash (Default)
NPHASE=3	Three-phase flash

PHASE..... Specifies the phase when NPHASE=1:

PHASE=V	Vapor (Default)
PHASE=L	Liquid
PHASE=S	Solid. Use for electrolytes system only.

FREE-WATER..... Use to override the free-water option established by the SIM-OPTIONS paragraph. (See Chapter 45.)

FREE-WATER=NO	Does not perform free-water calculations
FREE-WATER=YES	Performs free-water calculations

MAXIT..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

TOL ..... Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

T-EST ..... Temperature estimate used as an initial guess when the stream is flashed

P-EST ..... Pressure estimate used as an initial guess when the stream is flashed

BLOCK-OPTIONS Use to override diagnostic message levels for the history file and the terminal, established by the DIAGNOSTICS paragraph (see Chapter 45).

SIM-LEVEL ..... Sets the level of simulation errors and diagnostics printed in the history file (default is set by HISTORY SIM-LEVEL in the DIAGNOSTICS paragraph).

TERM-LEVEL..... Sets the level of simulation errors and diagnostics printed to the terminal (default is set by TERMINAL SIM-LEVEL in the DIAGNOSTICS paragraph)

VAR-LEVEL..... Sets the level of diagnostics printed in the history file for FORTRAN variables used in the DEFINE and VECTOR-DEF sentences (default is set by HISTORY VAR-LEVEL in the DIAGNOSTICS paragraph)

TVAR-LEVEL..... Sets the level of diagnostics printed to the terminal for FORTRAN variables used in the DEFINE and VECTOR-DEF sentences (default is set by TERMINAL VAR-LEVEL in the DIAGNOSTICS paragraph)

EO-OPTIONS Use to specify equation-oriented options for the Calculator.

COMPS ..... Component group for a list of components which can be active in this Calculator.

DERIV-METHOD ..... Preferred derivatives method, Analytic or Numeric. Update methods should not be used for Degree of Freedom run modes (Optimization or Reconciliation).

DERIV-METHOD = ANALYTICAL	Model derivatives (Jacobian) are determined from coded analytic expressions. Generally the preferred method.
DERIV-METHOD = NUMERICAL	Alternate method for calculating Jacobian. Useful when there is concern that analytic derivatives are causing convergence difficulties. Usually slower than analytic derivatives, more subject to precision issues. (Default)
DERIV-METHOD = UPDATE-ANALY	Use Schubert method for updating Jacobian, with analytic derivatives for the Base Jacobian. Use when Jacobian calculation is rate limiting step. May result in more iterations and be less robust than calculated derivatives.
DERIV-METHOD = UPDATE-NUMER	Use Schubert method for updating Jacobian, with numerical derivatives for the Base Jacobian. Use when Jacobian calculation is rate limiting step. May result in more iterations and be less robust than calculated derivatives.

SOLVE-METHOD ..... EO solution method. Specifies if open, closed, or neither method should be used with desired action and message level on failure.

SOLVE-METHOD= PERTURBATION	Closed solution method; use Perturbation layer around closed model. (Default)
SOLVE-METHOD= DO-NOT-CREAT	Ignore during EO solution.

INIT-ATTR Use to specify the attributes of open variables.

vname..... Name of the variable. (Required)

VALUE ..... Current value of the variable.

LOWER ..... Lower bound.

UPPER ..... Upper bound.

STEP ..... Step bound.

BOUND-TYPE ..... Bound type.

BOUND-TYPE = HARD	Do not violate the upper and/or lower bounds when solving a non-square (optimization or data regression) problem.
BOUND-TYPE = RELAXED	Relax upper and/or lower bound. If the initial value is outside the bound, set the bound to the initial value.
BOUND-TYPE = SOFT	Same as relaxed but add a penalty term to the objective to try to drive the value back to the bound.

SBWEIGHT ..... Soft bound weight.

PHYS-QTY ..... The physical quantity that the variable represents, for example, mole flow, temperature, or pressure. These types correspond to the standard Aspen Plus types.

UOM ..... Units of measure (standard Aspen Plus units), based on the physical type of the variable. Internally, all values are stored in SI units.

SCALE ..... Scale factor used by the solver.

SCRIPTS Use this sentence to specify scripts for a block.

METHOD ..... Script method. Blocks support default script methods of SETUP and INIT. User may define other methods. (Required)

TYPE ..... Type of script (Required)

TYPE = LOCALSCRIPT	Local Script
TYPE = GLOBALSCRIPT	Global Script
TYPE = FILE	File

LOCALSCRIPT ..... ID of a LOCAL SCRIPT paragraph. See Chapter 48.

GLOBALSCRIPT ..... ID of a GLOBAL SCRIPT paragraph. See Chapter 48.

FILE ..... Name of a file

32 Optimization

This chapter describes the input language for defining optimization and constraint specifications.

Use the OPTIMIZATION paragraph to:

- Identify the sampled flowsheet variables to be used in the objective function and equivalence them to FORTRAN variables using the DEFINE or VECTOR-DEF sentences.
- Specify the objective function as a function of the sampled variables using the MAXIMIZE or MINIMIZE sentence and optional inline FORTRAN statements.
- Identify the constraints associated with the optimization problem, using the CONSTRAINT paragraph.
- Identify the decision variables (feed stream and block input variables) that are to be varied to achieve the optimum by using the VARY sentence. An unlimited number of decision variables are allowed. However, you should keep this number to a minimum to avoid excessive computation time in solving the optimization problem.
- Supply upper and lower limits, and initial and maximum step sizes, for the decision variables. Use the LIMITS sentence.

Use the CONSTRAINT paragraph to:

- Identify the sampled flowsheet variables to be used in the constraint function and tolerance, and equivalence them to FORTRAN variables using the DEFINE or VECTOR-DEF sentences.
- Enter the constraint as a function of the sampled variables, using the SPEC sentence and optional inline FORTRAN statements.
- Supply a tolerance on the constraint, using the TOL-SPEC sentence.

Accessed flowsheet variables, except for VECTOR-DEF, are in units established by the IN-UNITS statement. You cannot use units options in brackets or braces.

CONSTRAINT and OPTIMIZATION Paragraphs

Input Language for CONSTRAINT and OPTIMIZATION

```
CONSTRAINT    conid
F             FORTRAN declaration statements
DEFINE    fvar    vartype    keyword=value
VECTOR-DEF    farray    vectype    keyword=value
F             Executable FORTRAN statements
SPEC    "expression1"    { LE | EQ | GE }    "expression2"
TOL-SPEC    "tol"
PARAM    keyword=value
```

Keywords for PARAM:

VECTOR INDEX1 INDEX2

```
OPTIMIZATION    optid
F             FORTRAN declaration statements
DEFINE    fvar    vartype    keyword=value
VECTOR-DEF    farray    STREAM    sid
F             Executable FORTRAN statements
{ MAXIMIZE "expression" | MINIMIZE "expression" }
CONSTRAINTS    conid / . . .
VARY    vartype    keyword=value
LIMITS    "lower"    "upper"    keyword=value
```

Optional keywords for LIMITS:

STEP-SIZE MAX-STEP-SIZE

Input Language Description for CONSTRAINT and OPTIMIZATION

conid..... Constraint ID

optid..... Optimization ID

DEFINE

Use to access a sampled flowsheet variable and equivalence it to the FORTRAN variable, *fvar*. The *fvar* variable is used in subsequent FORTRAN statements or expressions to represent the flowsheet variable. Sampled variables are in the input units in effect for the CONSTRAINT or OPTIMIZATION paragraph. Stream variables, stream properties, block input variables, and block results can be sampled. See Chapters 29 and 30 for a complete discussion of DEFINE statements.

VECTOR-DEF

Similar to DEFINE except that VECTOR-DEF equivalences an entire stream or block profile result to the FORTRAN array, *farray*. VECTOR-DEF is useful when several variables from the same array are needed. A CONSTRAINT or OPTIMIZATION paragraph must contain at least one DEFINE or VECTOR-DEF sentence. See Chapters 29 and 30 for a complete discussion of VECTOR-DEF statements.

FORTRAN statements Use to compute the constraint function and tolerance, the objective function, and manipulated variable limits. You need FORTRAN statements only if the functions involved are too complex to be represented by the SPEC, TOL-SPEC, MAXIMIZE, or MINIMIZE expressions. You can also use FORTRAN comments (not shown). See Chapter 31 and the *Aspen Plus User Guide* for a complete discussion of inline FORTRAN statements and expressions.

SPEC Use to define the constraint function. The constraint functions are defined as follows:

EQ For equality constraints: $expression1 - expression2 = 0$

LE For less than or equal to inequality constraints: $expression1 - expression2 \leq 0$

GE For greater than or equal to inequality constraints: $expression1 - expression2 \geq 0$

Where *expression1* and *expression2* are any valid FORTRAN arithmetic expressions, defined in the DEFINE sentence, and enclosed in quotes ("). Typically, *expression1* is a sampled flowsheet variable and *expression2* is a desired value or bound for the variable, in which case the quotes can be omitted. The SPEC sentence is required.

TOL-SPEC Use to enter the constraint tolerance:

EQ For equality constraints: $-tol < expression1 - expression2 < tol$

LE For less than or equal to inequality constraints: $expression1 - expression2 < tol$

GE For greater than or equal to inequality constraints: $expression1 - expression2 > -tol$

Where *tol* is any valid FORTRAN arithmetic expression enclosed in quotes ("). Typically, *tol* is a constant, in which case you can omit the quotes. The TOL-SPEC sentence is required.

PARAM Use to enter vector parameters to put constraints on vector variables for optimization problems. Constraint vectors are usually used for profiles, such as temperature profiles.

VECTOR Specifies if there is a vector constraint: YES or NO. (Default=NO)

INDEX1 First element of the constraint vector. You must specify VECTOR=YES. (Default=1)

INDEX2 Last element of the constraint vector. You must specify VECTOR=YES.

MAXIMIZE, MINIMIZE Use to specify the objective function for the optimization problem. *expression* is any valid FORTRAN arithmetic expression enclosed in quotes ("). The OPTIMIZATION paragraph must contain one MAXIMIZE or one MINIMIZE sentence.

CONSTRAINTS Use to specify any constraint associated with the optimization problem.

conid Constraint ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

VARY Use to identify decision variables. Only block input or process feed stream variables can be decision variables. Integer block input variables, such as the feed location of a distillation column, cannot be decision variables. The initial guess used for a decision variable is the stream or block input specification for the variable. You must enter one VARY sentence and one LIMITS sentence for each decision variable. An optimization problem can contain any number of decision variables. See Chapter 29 for a complete discussion of the VARY sentence.

LIMITS

Use to specify limits for the decision variable, where *lower* and *upper* are any valid FORTRAN arithmetic expressions enclosed in quotes ("). LIMITS expressions are evaluated before the first iteration of the optimization convergence loop. They are not re-evaluated before subsequent iterations. Typically, the limits are constants, in which case you can omit the quotes. The LIMITS sentence is required. You can also use the LIMITS sentence to enter initial step size and maximum step size:

STEP-SIZE..... Initial step size for the decision variable. The step size is based on the option selected for STEP-OPT in the CONV-OPTIONS SQP sentence or the CONVERGENCE paragraph in the PARAM sentence. Values entered in a CONVERGENCE paragraph supersede values entered in the OPTIMIZATION paragraph.

MAX-STEP-SIZE ..... Maximum step size for the decision variable. The step size is defined as a fraction of the range (upper limit minus lower limit). Values entered in a CONVERGENCE paragraph supersede values entered in the OPTIMIZATION paragraph.

33 Transfer Blocks

This chapter describes the input language for TRANSFER blocks.

Use the TRANSFER block to copy the values of flowsheet variables from one part of the flowsheet to another. You can transfer streams, stream variables, and block variables. The most common application is to copy one stream into another.

If the transferred variable is a stream variable, you can also supply the thermodynamic condition of the destination stream.

TRANSFER Block Paragraph

Input Language for TRANSFER

```
TRANSFER    tblockid
SET    vartype    keyword=value
SET    STREAM    sid
SET    STREAM-FLOWS    sid
SET    SUBSTREAM    STREAM=sid    SUBSTREAM=ssid
EQUAL-TO    vartype    keyword=value
EQUAL-TO    STREAM    sid
EQUAL-TO    STREAM-FLOWS    sid
EQUAL-TO    SUBSTREAM    STREAM=sid    SUBSTREAM=ssid
EXECUTE    executionopt    blocktype    blockid
```

Executionopts:

FIRST LAST BEFORE AFTER

Blocktypes:

BLOCK CONVERGENCE TRANSFER CALCULATOR BALANCE PRES-RELIEF

```
FLASH-SPECS    sid    kode    keyword=value
```

Keywords:

TEMP PRES VFRAC

Optional keywords:

NPHASE PHASE FREE-WATER MAXIT TOL T-EST P-EST

```
BLOCK-OPTIONS    keyword=value
```

Keywords:

SIM-LEVEL TERM-LEVEL

Input Language Description for TRANSFER

tblockid..... Transfer block ID

SET Use to identify the scalar stream or block variable into which a scalar variable is copied. This form of SET has the same syntax as the VARY sentence. (See Chapter 29.)

vartype ..... Variable type. You can use any variable type allowed for the VARY sentence. (See Chapters 29 and 30.)

SET STREAM Use to identify the stream into which a whole stream is copied.

sid..... Stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

SET STREAM-FLOWS Use to identify the stream into which the component flows and the total flow of a stream is copied.

sid..... Stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

SET SUBSTREAM Use to identify the stream into which the substream of a stream is copied.

sid..... Stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

ssid..... Substream ID

EQUAL-TO

Use to identify a flowsheet variable from which information is copied. EQUAL-TO has the same syntax as SET. Any number of SET sentences can be followed by a single EQUAL-TO sentence. This allows you to transfer information from the same flowsheet variable to variables within other parts of the flowsheet. All SET and EQUAL-TO sentences must be of the same form. The form must be one of the following: SET *vartype*, SET STREAM, SET STREAM-FLOWS, or SET SUBSTREAM. When you use the SET *vartype* form, the *vartype* within each SET sentence does not have to be the same, but it must have the same physical dimension (such as temperature).

EXECUTE

Use to specify when the transfer block is executed. A transfer block can have only one EXECUTE sentence. If you enter the transfer block ID in a user-supplied sequence, the EXECUTE sentence is not required.

executionopt..... Execution options:

FIRST	Transfer block executed at beginning of simulation
LAST	Transfer block executed at end of simulation
BEFORE	Transfer block executed before a block specified by *blocktype* and *blockid*
AFTER	Transfer block executed after a block specified by *blocktype* and *blockid*

blocktype..... Block type. Use only for BEFORE and AFTER execution options.

BLOCK	Unit operation block
CONVERGENCE	Convergence block
TRANSFER	Transfer block
CALCULATOR	Calculator block
BALANCE	Balance block
PRES-RELIEF	Pressure relief block

blockid..... Block ID of the specified *blocktype*. Use only for BEFORE and AFTER execution options.

FLASH-SPECS

Use to specify the thermodynamic condition of a stream modified by a transfer block. Or use to request or suppress flash calculations. FLASH-SPECS is frequently used to supply temperature, pressure, vapor fraction, or flash options, for streams assigned material flows using the SET STREAM-FLOWS form of SET.

If you do not use FLASH-SPECS, Aspen Plus decides whether or not to flash the stream. Aspen Plus:

- Does not flash a stream if the only transferred variables are total flow, enthalpy, entropy, or density
- Flashes a stream if the temperature, pressure, or composition of the stream is transferred

If Aspen Plus determines that a flash is necessary, it uses the values present in the stream, and the flash options established in the STREAM paragraph or source block of the stream.

sid..... Stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

kode..... Thermodynamic condition of flash calculation:

NOFLASH	Stream is not flashed
PH	PH flash
TP	TP flash
PV	PV flash

	TH	TH flash
	TV	TV flash

TEMP Temperature. Allowed only when *kode* is TP, TH, or TV. (Default=value present in the stream)

PRES Pressure. Allowed only when *kode* is PH, TP, or PV. (Default=value present in the stream)

VFRAC Vapor fraction. Allowed only when *kode* is PV or TV. (Default=value present in the stream)

NPHASE Number of phases in MIXED substream:

NPHASE=1	One-phase calculation
NPHASE=2	Two-phase flash (Default)
NPHASE=3	Three-phase flash

PHASE Specifies the phase when NPHASE=1:

PHASE=V	Vapor (Default)
PHASE=L	Liquid
PHASE=S	Solid. Use for electrolytes system only.

FREE-WATER Use to override the free-water option established by the SIM-OPTIONS paragraph. (See Chapter 45.)

FREE-WATER=NO	Does not perform free-water calculations
FREE-WATER=YES	Performs free-water calculations

MAXIT Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

TOL Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

T-EST Temperature estimate. Use to aid flash convergence when *kode* is PH or PV.

P-EST Pressure estimate. Use to aid flash convergence when *kode* is TH or TV.

BLOCK-OPTIONS Use to override the diagnostic message levels established by the DIAGNOSTICS paragraph. (See Chapter 45.)

34 Balance Blocks

This chapter describes the input language for BALANCE blocks.

Use the BALANCE block to:

- Calculate feed stream flow rate and conditions, based on other stream and block information. This can eliminate the need for DESIGN-SPECs and convergence loops.
- Calculate the flow rate of make-up streams in recycle calculations. The BALANCE block can eliminate Calculator blocks for this purpose.

BALANCE Block

Input Language for BALANCE

```
BALANCE    balanceid
DESCRIPTION  "a balance description - up to 64 characters in quotes"
PARAM      keyword=value
```

Optional keywords:

EXECUTE NMOLE NMASS CHECK MAXIT TOL XTOL

```
M-BAL    mbalno    keyword=value
```

Keywords:

BLOCKS INLETS OUTLETS COMPS SUBSTREAM

```
E-BAL    eblano    keyword=value
```

Keywords:

BLOCKS INLETS OUTLETS RHS

```
SCALE    sid    scalefactor
MOLE-EQN    eqno    termno    sid    ssid    cid    coef  / . . .
MOLE-RHS    eqno    molerhs
MASS-EQN    eqno    termno    sid    ssid    cid    coef  / . . .
MASS-RHS    eqno    massrhs
CALCULATE    sid    keyword=value  / . . .
```

Keywords:

FLOW ENTHALPY COMPS SUBSTREAM UPDATE

```
EXECUTE    executionopt    blocktype    blockid
```

Executionopts:

FIRST LAST BEFORE AFTER

Blocktypes:

BLOCK CONVERGENCE TRANSFER CALCULATOR BALANCE

```
FLASH-SPECS    sid    kode    keyword=value
```

Keywords:

TEMP PRES VFRAC

Optional keywords:

NPHASE PHASE MAXIT TOL FREE-WATER T-EST P-EST

```
BLOCK-OPTIONS    keyword=value
```

Optional keywords:

SIM-LEVEL TERM-LEVEL STREAM-LEVEL

Input Language Description for BALANCE

balanceid ..... Balance block ID

DESCRIPTION A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the BALANCE block report.

PARAM Use to enter execution options and optional convergence parameters.

EXECUTE ..... Specifies how often the BALANCE block should be executed if the BALANCE block is inside a convergence loop.

EXECUTE=ONCE	Executes only on the first iteration of the loop
EXECUTE=ALWAYS	Executes every iteration of the loop (Default)
EXECUTE=NEVER	Skips BALANCE execution

NMOLE ..... Number of mole equations

NMASS ..... Number of mass equations

CHECK ..... Specifies correction actions when implicit BALANCE equations are not satisfied. Implicit equations are equations that have not been explicitly specified by E-BAL or M-BAL. (For example, if E-BAL is specified the mass balance equations are the implicit equations.)

CHECK=SKIP-BLOCK	Skips the balance block. Does not update calculated variables. (Default)
CHECK=NONE	Does not check implicit balance equations
CHECK=PROCEED	Continues to update calculated variables, even with errors

MAXIT ..... Maximum number of iterations allowed for BALANCE calculations (Default=30)

TOL ..... Relative tolerance of balance equation residuals (Default=$1x10^{-4}$)

XTOL ..... Alternative tolerance when convergence cannot be achieved because one or more variables have reached their upper or lower limits. A solution is found that minimizes the sum of squares of design specification, and tear stream errors divided by their respective tolerances. Iterations stop when the root-mean-square of the changes in the scaled manipulated variables is less than XTOL. Each manipulated variable is scaled by dividing by the absolute value of the lower or upper limit, whichever is larger. (Default=$1x10^{-4}$)

M-BAL Use to specify mass balance equations. You must specify either the blocks or the inlet and outlet streams to be included in the material balance envelope.

mbalno ..... Mass balance equation number

BLOCKS ..... IDs of Blocks to be included in the material balance envelope. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

INLETS ..... Inlet stream IDs for the material balance envelope. You must also specify OUTLETS. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

OUTLETS ..... Outlet stream IDs for the material balance envelope. You must also specify INLETS. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

COMPS ..... Component IDs or component group IDs. Balance calculations are performed for each of the substream/component combinations.

SUBSTREAM ..... Substream IDs. Balance calculations are performed for each of the substream/component combinations.

E-BAL Use to specify energy balance equations. You must specify either the blocks or the inlet and outlet streams to be included in the energy balance envelope.

ebalno..... Energy balance equation number

BLOCKS..... IDs of Blocks to be included in the energy balance envelope. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

INLETS..... Inlet stream IDs for the energy balance envelope. You must also specify OUTLETS. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

OUTLETS ..... Outlet stream IDs for the energy balance envelope. You must also specify INLETS. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

RHS..... Right-hand side value for the energy balance equation (Default=0)

SCALE Use to change the values of stream component flows.

sid..... Stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

scalefactor ..... Stream scale factor. Stream is multiplied by this factor before balance calculations.

MOLE-EQN Use to set up mole equations among the total or component molar flows over multiple components of multiple streams.

eqno ..... Mole equation number

termno..... Sequence number of the term on the left-hand side

sid..... Stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

ssid ..... Substream ID

cid..... Component ID

coef..... Coefficient for mole flow quantity

MOLE-RHS Use to specify the right-hand side for a mole equation.

eqno ..... Mole equation number

molerhs ..... Right-hand side for the mole equation (Default=0)

MASS-EQN Use to set up mass equations among the total or component mass flows over multiple components in multiple streams.

eqno ..... Mass equation number

termno..... Sequence number of the term on the left-hand side

sid..... Stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

ssid ..... Substream ID

cid..... Component ID

coef..... Coefficient for mass flow quantity

MASS-RHS Use to specify the right-hand side for a mass equation.

eqno ..... Equation number

massrhs ..... Right-hand side for the mass equation (Default=0)

CALCULATE

Use to calculate and update stream variables after the mass and energy balance relationships have been solved.

sid..... Stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

FLOW ..... Type of flow variable to be calculated:

FLOW=TOTAL	Calculates total flow. Stream composition remains the same.
FLOW=SUBS	Calculates substream flows. Stream composition remains the same.
FLOW=COMPS	Calculates component flows
FLOW=NONE	Does not calculate any flows. Only calculates an energy balance.

ENTHALPY..... Switch to calculate enthalpy: YES or NO

COMPS ..... Components for which flows are to be calculated. You must also specify ENTHALPY and FLOW=COMPS.

SUBSTREAM ..... Substream ID. You must also specify FLOW=SUBS or FLOW=COMPS.

UPDATE..... Switch to update calculated variables: YES or NO (Default=YES)

EXECUTE

Use to specify when the balance block is executed. A balance block can have only one EXECUTE sentence. If the balance block ID is entered in a user-supplied sequence, the EXECUTE sentence is not required.

executionopt..... Execution options:

FIRST	Balance block executed at beginning of simulation
LAST	Balance block executed at end of simulation
BEFORE	Balance block executed before a block, specified by *blocktype* and *blockid*
AFTER	Balance block executed after a block, specified by *blocktype* and *blockid*

blocktype ..... Block type. Use only for BEFORE and AFTER execution options.

BLOCK	Unit operation block
CONVERGENCE	Convergence block
TRANSFER	Transfer block
CALCULATOR	Calculator block
BALANCE	Balance block

blockid ..... Block ID of the specified *blocktype*. Use only for BEFORE and AFTER execution options.

FLASH-SPECS

Use to specify thermodynamic conditions for streams updated by a balance block. Or use to either request or suppress flash calculations for those streams. If you do not enter FLASH-SPECS, Aspen Plus automatically flashes an updated stream, except when the only updated variable is total flow.

sid..... Stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

kode..... Thermodynamic condition of flash calculation:

NOFLASH	Does not perform flash calculation for this stream
PH	PH flash
TP	TP flash

	PV	PV flash
	TH	TH flash
	TV	TV flash

TEMP Stream temperature. Allowed only when *kode* is TP, TH, or TV. (Default=value present in the stream)

PRES Stream pressure. Allowed only when *kode* is PH, PV, or TP. (Default=value present in the stream)

VFRAC Stream vapor fraction. Allowed only when *kode* is PV, or TV. (Default=value present in the stream)

NPHASE Number of phases in a MIXED substream:

NPHASE=1	One-phase calculation
NPHASE=2	Two-phase flash (Default)
NPHASE=3	Three-phase flash

PHASE Specifies the phase when NPHASE=1:

PHASE=V	Vapor (Default)
PHASE=L	Liquid
PHASE=S	Solid. Use for electrolytes system only.

MAXIT Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

TOL Flash convergence tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

FREE-WATER Use to override the free-water option established by the SIM-OPTIONS paragraph. (See Chapter 45.)

FREE-WATER=NO	Does not perform free-water calculations
FREE-WATER=YES	Performs free-water calculations

T-EST Temperature estimate. Use to aid flash convergence when *kode* is PH or PV.

P-EST Pressure estimate. Use to aid flash convergence when *kode* is TH or TV.

BLOCK-OPTIONS Use to override the diagnostic message levels established by the DIAGNOSTICS paragraph. (See Chapter 45.)

Accessing Variables in BALANCE

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following table lists variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variable	ID1	ID2
PARAM	EXECUTE	—	—
E-BAL	RHS	ebalno	—
SCALE	SCALE	sid	—
MOLE-EQN	COEF	eqno	termno
MASS-EQN	COEF	eqno	termno

35 Sensitivity Blocks

This chapter describes the input language for defining sensitivity blocks.

Use the SENSITIVITY paragraph to:

- Identify the flowsheet variables to be tabulated or to be used in FORTRAN expressions or inline FORTRAN statements, and equivalence them to FORTRAN variables using the DEFINE or VECTOR-DEF sentences.
- Select or compute the variables to be tabulated, using the TABULATE sentence and optional inline FORTRAN statements.
- Identify the feed stream or block input variables to be varied to generate the table, using the VARY sentence. Sensitivity blocks can have up to five varied variables when the plot sentence is not included. When you request plots, only one VARY sentence is allowed.

You can use the SENSITIVITY paragraph to select values for each variable to be varied. You can select values by entering:

- A list of values.
- Lower and upper limits. Then enter either the number of equally-spaced points between the limits or the size of the increment between points. Use the RANGE statement for this purpose.

SENSITIVITY Block Paragraph

Input Language for SENSITIVITY

```
SENSITIVITY    sblockid
DESCRIPTION    "a sensitivity description - up to 64 characters in quotes"
F              FORTRAN    declaration statements
DEFINE    fvar    vartype    keyword=value
VECTOR-DEF    farray    vectype    keyword=value
F              Executable FORTRAN statements
TABULATE    colno    "expression"    COL-LABEL="line1". . ."line4"    &
       UNIT-LABEL="line5"    "line6"
VARY    vartype    keyword=value
RANGE    keyword=value
```

Keywords:

LIST LOWER UPPER NPOINT INCR

REINIT BLOCKS = { **ALL** / **blockid – list** } **STREAMS =** { **ALL** / **sid – list** }

PLOT *keyword=value*

Optional keywords:

COLUMNS X-AXIS X-SCALE Y-SCALE PLOT-HEADING
WIDE GRID INTERPOLATE

PARAM *keyword=value*

Optional keywords:

WIDE HIGH-PRECISION BASE-CASE

BLOCK-OPTIONS *keyword=value*

Keywords:

VAR-LEVEL TVAR-LEVEL

Input Language Description for SENSITIVITY

sblockid ..... Sensitivity block ID

DESCRIPTION A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the SENSITIVITY block report.

DEFINE, VECTOR-DEF Use to access a flowsheet variable and equivalence it to the FORTRAN variable *fvar*, which is used in the subsequent FORTRAN statements or the TABULATE or RANGE expressions to represent the flowsheet variable. VECTOR-DEF is similar to DEFINE except that VECTOR-DEF equivalences an entire stream or block profile results to the FORTRAN array, *farray*. A SENSITIVITY paragraph must contain at least one DEFINE or VECTOR-DEF sentence. See Chapters 29 and 30 for a complete discussion of the DEFINE and VECTOR-DEF sentences.

FORTRAN statements A FORTRAN statement is any valid FORTRAN statement subject to the restrictions discussed in the *Aspen Plus User Guide*. You can use FORTRAN comments (not shown). FORTRAN statements are needed only if the tabulated results or RANGE values are too complex to be represented by the TABULATE and RANGE expressions.

TABULATE Use to define the tabulated results. Enter one TABULATE sentence for each tabulated result, to generate one column in the sensitivity table. You can also use TABULATE to supply column headings for tabulated results. Column headings consist of six lines of eight characters each. The first four lines (COL-LABEL) identify the tabulated results. The last two lines (UNIT-LABEL) display the units of tabulated results. If the tabulated results expression is a single FORTRAN variable defined by a DEFINE sentence, then Aspen Plus automatically generates UNIT-LABEL. Otherwise, you must enter the UNIT-LABEL or leave it blank.

colno	Table column number. Column number 1 is the first column after the columns for the varied variables.
expression	Any valid FORTRAN arithmetic expression enclosed in quotes ("). It is used to compute the tabulated values. Typically, *expression* is a single FORTRAN variable name, in which case you can omit the quotes.
line1. . .line4	Column heading used to identify tabulated results. A string of up to eight characters enclosed in quotes (").
line5. . .line6	Column heading used to display units of tabulated results. A string of up to eight characters enclosed in quotes (").

VARY Use to identify the flowsheet variables that are to be varied to generate the table. Only block input and process feed stream variables can be varied. You must enter one VARY sentence and one RANGE sentence for each varied variable. A sensitivity block can have up to five VARY and RANGE sentences when a PLOT sentence is not included. When you request plotting, only one VARY sentence is allowed. See Chapters 29 and 30 for a complete discussion of the VARY sentence.

RANGE Use to specify values for the varied variables. Aspen Plus generates one row of the table for each possible combination of varied variable values. You can use only one of the keywords LIST, NPOINT, INCR in a RANGE statement.

LIST	List of varied variable values
LOWER	Lower limit of the varied variable range. It can be a constant or FORTRAN expression in terms of FORTRAN variables.
UPPER	Upper limit of the varied variable range. It can be a constant or FORTRAN expression in terms of FORTRAN variables.
NPOINT	Number of points including LOWER and UPPER. It can also be any valid FORTRAN arithmetic expression in quotes.
INCR	Increment size between intermediate points. It can also be any valid FORTRAN arithmetic expression in quotes.

REINIT Use to reset convergence and unit operation restart flags. (See Chapter 45.) Also use to restore tear streams or streams manipulated by design specifications or by FORTRAN blocks to their initial values, and to reset any other flowsheet stream to zero flow.

Normally, REINIT is not used, since it is usually most efficient to begin calculations for a new row evaluation with the results of the previous row evaluation.

blockid-list	List of convergence and unit operation blocks for which the restart feature is suppressed when a new row evaluation begins. When restart is suppressed for a block, the initialization algorithm for the convergence method or unit operation model is invoked at the beginning of each row evaluation. IDs can be hierarchical; see Chapter 9 for naming conventions and restrictions. Enter ALL to reinitialize all blocks. (Default=no blocks are reinitialized)

	sid-list		List of streams whose initial values are restored when a new row evaluation begins. IDs can be hierarchical; see Chapter 9 for naming conventions and restrictions. Enter ALL to reinitialize all streams. (Default=no streams are reinitialized)
PLOT	Use to generate print-plots of sensitivity block results. Only one VARY sentence is allowed when plots are produced. The variable named in the X-AXIS keyword is the independent variable for the plots. The column numbers specified in the PLOT sentence are the dependent variables for the plots. Up to five columns can be placed on a single plot. If you list more than five columns in a PLOT sentence, Aspen Plus will produce multiple plots.		
	COLUMNS		List of column numbers from the TABULATE sentences for the dependent variables to be plotted. (Default=all columns)
	X-AXIS		Column number from the TABULATE sentence to be used as the independent variable for the plots. (Default=variable named in VARY sentence)
	X-SCALE	**X-SCALE=STANDARD**	Uses linear scale on horizontal axis of plots (Default)
		X-SCALE=INVERSE	Uses inverse scale on horizontal axis of plots
	Y-SCALE	**Y-SCALE=STANDARD**	Uses linear scale on vertical axis of plots (Default)
		Y-SCALE=INVERSE	Uses inverse scale on vertical axis of plots
		Y-SCALE=LOG	Uses logarithmic scale on vertical axis of plots
	PLOT-HEADING		Heading up to 64 characters included in quotes, printed at the top of the print-plot
	WIDE, GRID, INTERPOLATE		Plot options. Use to override the defaults established by the PLOT-OPTIONS paragraph. (See Chapter 46.)
PARAM	Use to specify the format of the table of results and execution options.		
	WIDE	**WIDE=NO**	Generated tables are limited to 80 columns wide (Default)
		WIDE=YES	Generated tables are greater than 80 columns wide
	HIGH-PRECISION	**HIGH-PRECISION=YES**	Prints seven significant digits
		HIGH-PRECISION=NO	Prints five significant digits (Default)
	BASE-CASE		Base-case execution options:
		BASE-CASE=LAST	Executes base-case last (Default)
		BASE-CASE=FIRST	Executes base-case first
		BASE-CASE=NO	Does not execute base-case
BLOCK-OPTIONS	Use to override diagnostic message levels for the history file and the terminal, established by the DIAGNOSTICS paragraph (see Chapter 45).		
	VAR-LEVEL		Sets the level of diagnostics printed in the history file for FORTRAN variables that are used in the DEFINE and VECTOR-DEF sentences (default is set by HISTORY-VAR-LEVEL in the DIAGNOSTICS paragraph).
	TVAR-LEVEL		Sets the level of diagnostics printed to the terminal for FORTRAN variables that are used in the DEFINE and VECTOR-DEF sentences (default is set by TERMINAL VAR-LEVEL in the DIAGNOSTICS paragraph).

36 Case-Study Blocks

This chapter describes the input language for CASE-STUDY blocks.

Use the CASE-STUDY paragraph to:

- Identify flowsheet variables that are to be changed from case to case by using the VARY sentence.
- Assign case values for each variable by using the CASE sentence.
- Supply case report options if they are different from the default report options. An Aspen Plus input file can have only one case-study block.

CASE-STUDY Block Paragraph

Input Language for CASE-STUDY

```
CASE-STUDY
VARY    vartype    keyword=value
CASE    caseno     value-list    REINIT-BLOCKS = { ALL | blockid – list }  &
        EINIT-STREAMS = { ALL | sid – list }

DESCRIPTION    caseno    "a case study description - up to 64 characters in quotes"
        REPORT    reportopt-list
```

Reportopts:

NOREPORT INPUT NOFLOWSHEET NOSENSITIVITY NOPROPERTIES NOBLOCKS NOSTREAMS

```
FLOWSHEET-REPORT    reportopt-list
```

Reportopts:

NODESCRIPTION NOTOTBAL NOCONVERGENCE NOCOMPBAL NOSEQUENCE NOFORTRAN NODESIGN-SPEC NOCONSTRAINT NOOPTIMIZATION NOTRANSFER

```
BLOCK-REPORT    INCL-BLOCKS=blockid-list    EXCL-BLOCKS=blockid-list
STREAM-REPORT    reportopt-list    PROPERTIES=propsetid-list  &
        INCL-STREAMS=sid-list    EXCL-STREAMS=sid-list
SUP-STREAM-REPORT    supno    reportopt-list    PROPERTIES=propsetid-list  &
        INCL-STREAMS=sid-list    EXCL-STREAMS=sid-list
```

Reportopts:

NOREPORT WIDE NOSORT NOZEROFLOW NOMOLEFLOW MASSFLOW STDVOLFLOW MOLEFRAC MASSFRAC STDVOLFRAC

Input Language Description for CASE-STUDY

VARY

Use to identify the variables that are to be changed from case to case. You can only change block input and process feed stream variables. Enter one VARY sentence for each case-study variable. See Chapters 29 and 30 for a complete discussion of the VARY sentence.

CASE

Use to specify the values for the case-study variables. In addition, you can use REINIT-BLOCKS to reset convergence and unit operation restart flags. (See Chapter 45.) You can use REINIT-STREAMS to restore tear streams or feed streams manipulated by design specifications or by Calculator blocks to their initial values. You can also use REINIT-STREAMS to reset any other flowsheet stream to zero flow. Normally you do not use these keywords, because it is more efficient to begin the calculations for a new case with the results of the previous case. Enter one CASE sentence for each case to be evaluated in addition to the base case.

caseno ..... Case number

value-list ..... List of values for the case-study variables, in the same order as the VARY sentences. Values are in the units established by the IN-UNITS statement. You cannot use unit options in brackets or braces.

blockid-list..... List of block IDs. Enter ALL to reinitialize all blocks. By default no blocks are reinitialized. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

sid-list ..... List of stream IDs. Enter ALL to reinitialize all streams. By default no streams are reinitialized. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

DESCRIPTION

A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the CASE-STUDY paragraph report.

caseno ..... Case number

REPORT, FLOWSHEET-REPORT, BLOCK-REPORT, STREAM-REPORT, SUP-STREAM-REPORT

Use to specify report options for the case-study reports. (The PROPERTY report is automatically suppressed in case-study reports.) The only report option discussed in Chapter 46 that cannot be used in the case-study block is REPORT-SCALE. Report scaling specifications apply to all case-study cases and to the base case. The REPORT, FLOWSHEET-REPORT, and BLOCK-REPORT sentences are used in the same way as the corresponding paragraphs described in Chapter 46. The STREAM-REPORT and SUP-STREAM-REPORT sentences are used in the same way as the STREAM-REPORT paragraph described in Chapter 46. If you specify report options for the base case and would like the same options for the case-study reports, you must respecify the report options in the CASE-STUDY paragraphs. All other keywords are also described in Chapter 46.

37 Flowsheet Convergence

This chapter describes the input language for entering flowsheet convergence specifications. Flowsheets with recycle loops, design specifications, or optimization problems must be solved iteratively. The iterative solution requires the determination of the tear streams, tear variables, convergence methods, and calculation sequence. Aspen Plus performs all these functions automatically. However, you can supply part or all of the convergence specifications, using the input language in this chapter.

The specifications are:

- User-specified convergence options.
- User-selected tear streams.
- User-generated convergence blocks.
- Convergence plots.
- User-supplied calculation sequence.

In most cases you will find the default action satisfactory and will not need to supply specifications.

User-Specified Convergence Options

Input Language for CONV-OPTIONS

```
CONV-OPTIONS
PARAM    keyword=value
```

Optional keywords:

TEAR-METHOD TOL COMPS STATE TRACE UPDATE FLASH TRACEOPT SPEC-METHOD OPT-METHOD COMB-METHOD MSPEC-METHOD SPEC-LOOP USER-LOOP TEAR-VAR TEAR-WEIGHT LOOP-WEIGHT CHECKSEQ AFFECT

```
WEGSTEIN    keyword=value
```

Optional keywords:

MAXIT WAIT QMIN QMAX ACCELERATE NACCELERATE

```
DIRECT    MAXIT=value
SECANT    keyword=value
```

Optional keywords:

MAXIT STEP-SIZE MAX-STEP-SIZE XTOL BRACKET XFINAL STOP

```
BROYDEN    keyword=value
```

Optional keywords:

MAXIT WAIT XTOL TEAR-TOL TEAR-RATIO TEAR-MAXIT QMIN QMAX

```
NEWTON    keyword=value
```

Optional keywords:

MAXIT MAXPASS WAIT REINIT RED-FACTOR XTOL TEAR-TOL TEAR-RATIO TEAR-MAXIT QMIN QMAX

```
SQP    keyword=value
```

Optional keywords:

MAXIT MAXPASS WAIT TOL QMIN QMAX MAXLSPASS NLIMIT PRINT-PLOT STEP-OPT STEP-DIR OPT-METHOD DERIVATIVE EST-STEP CONST-ITER DERIV-SWITCH STEP-PRES STEP-ENTH STEP-FLOW STEP-HEAT VAR-MIN CONV-TEST

Input Language Description for CONV-OPTIONS

Use the CONV-OPTIONS paragraph to specify convergence parameters and/or methods for both system-generated and user-generated convergence blocks.

PARAM

Use to specify convergence methods, tear tolerance and convergence variables, and tearing and sequencing parameters.

TEAR-METHOD ..... Tear stream convergence method. See User-Generated Convergence Blocks, this chapter, for guidance on selecting convergence methods.

TEAR-METHOD=WEGSTEIN	Wegstein method (Default)
TEAR-METHOD=DIRECT	Direct substitution method
TEAR-METHOD=BROYDEN	Broyden method
TEAR-METHOD=NEWTON	Newton method

TOL ..... Tear stream convergence tolerance (Default=$1x10^{-4}$)

COMPS ..... Component group ID. The component group should consist of a list of components to be converged in the tear stream. (See Note 5.) (Default=all components)

STATE ..... State variables to be converged. (See Note 5.)

STATE=PH	Pressure and enthalpy (Default)
STATE=P	Pressure
STATE=H	Enthalpy
STATE=NONE	No state variables are converged

TRACE ..... Trace component threshold. The convergence test is bypassed for components whose mole fraction is less than TRACE. (Default=*tol*/100)

UPDATE.....

UPDATE=YES	Updates tear streams on the last iteration if the convergence block does not converge
UPDATE=NO	Does not update tear streams on the last iteration (Default)

FLASH .....

FLASH=YES	Flashes tear streams after being updated by the convergence block (Default)
FLASH=NO	Does not flash tear streams after update

TRACEOPT..... Convergence test options for trace component:

TRACEOPT=CUTOFF	Ignores convergence test for trace component (Default)
TRACEOPT=GRADUAL	Gradually relaxes convergence criterion for trace component

SPEC-METHOD ..... Convergence method for single design specification convergence:

SPEC-METHOD=SECANT	Secant method (Default)
SPEC-METHOD=BROYDEN	Broyden method
SPEC-METHOD=NEWTON	Newton method

OPT-METHOD ..... Convergence method for optimization:

OPT-METHOD=SQP	Sequential quadratic programming (Default)
OPT-METHOD=COMPLEX	Complex method

COMB-METHOD ..... Convergence method for combined tear streams and design specification convergence:

COMB-METHOD=BROYDEN	Broyden method (Default)
COMB-METHOD=NEWTON	Newton method

MSPEC-METHOD..... Convergence method for multiple design specification method:

	MSPEC-METHOD= BROYDEN	Broyden method (Default)
	MSPEC-METHOD= NEWTON	Newton method
SPEC-LOOP	Specifies how system should converge design specifications:	
	SPEC-LOOP=INSIDE	Converges design specifications individually. Nests the design specification convergence loops inside tear stream convergence loops. (Default)
	SPEC-LOOP=OUTSIDE	Converges design specifications individually. Nests the design specification convergence loops outside tear stream convergence loops.
	SPEC-LOOP=IN-SIMUL	Converges multiple design specifications in the same subsystem simultaneously. Nests the design specification convergence loops inside tear stream convergence loops.
	SPEC-LOOP=OUT-SIMUL	Converges multiple design specifications in the same subsystem simultaneously. Nests the design specification convergence loops outside tear stream convergence loops.
	SPEC-LOOP= WITH-TEARS	When both tear streams and design specifications are in the same subsystem, converge them simultaneously.
USER-LOOP	Specifies where to place user-provided convergence blocks in relation to system-generated convergence blocks:	
	USER-LOOP=OUTSIDE	Nests convergence blocks in CONV-ORDER outside other convergence blocks when both types of convergence blocks are present in the same subsystem (Default)
	USER-LOOP=INSIDE	Nests convergence blocks in CONV-ORDER inside other convergence blocks when both types of convergence blocks are present in the same subsystem
TEAR-VAR	**TEAR-VAR=YES**	Tears Calculator block WRITE-VARS. (See Chapter 31.)
	TEAR-VAR=NO	Does not tear Calculator block WRITE-VARS (Default)
TEAR-WEIGHT	Relative weighting given to stream tearing. Tearing algorithm would minimize tear variables with large TEAR-WEIGHT. (Default=1)	
LOOP-WEIGHT	Relative weighting given to loop tearing. Tearing algorithm would minimize loops torn with large LOOP-WEIGHT. (Default=1)	
CHECKSEQ	Specifies whether to treat missing tear streams or tear variables as error or warning	
	CHECKSEQ=YES	Issues error message when a tear stream is missing from user defined sequence (Default)
	CHECKSEQ=NO	Issues warning message when a tear stream is missing from user defined sequence
AFFECT	Specifies whether to use logic to determine which blocks can be affected by changed inputon an edit run.	
	AFFECT=YES	Only reruns blocks with changed input and other blocks whose results can be affected. (Default)
	AFFECT=NO	Reruns all blocks in the calculation sequence after the first block with changed input.

WEGSTEIN, DIRECT, SECANT, BROYDEN, NEWTON, SQP

Use to enter convergence parameters for each method. The keywords are defined in the description of each method later in this chapter.

User-Selected Tear Streams

Input Language for TEAR

TEAR	**sid**	**[tol]**	*keyword=value*	**/ . . .**

Optional keywords:

COMPS STATE TRACE

Input Language Description for TEAR

Use the TEAR paragraph to designate streams as preferred tear streams and, optionally, the variables to be converged in the tear stream. Aspen Plus will automatically generate convergence blocks and calculation sequence. The TEAR paragraph is non-hierarchical, but you can specify streams inside hierarchies.

sid ..... Tear stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

tol ..... Tear stream convergence tolerance (Default=$1x10^{-4}$ or value specified in CONV-OPTIONS paragraph)

COMPS ..... Component group ID. The component group should consist of a list of components to be converged in the tear stream. Defaults are established by the CONV-OPTIONS paragraph. (See Note 5.)

STATE ..... State variables to be converged. (See Note 5.)

STATE=PH	Pressure and enthalpy (Default)
STATE=P	Pressure
STATE=H	Enthalpy
STATE=NONE	No state variables are converged

TRACE ..... Trace component threshold. The convergence test is bypassed for components whose mole fraction is less than TRACE. (Default=*tol*/100)

User-Generated Convergence Blocks

You can use convergence blocks to converge tear streams, tear variables, design specifications, and/or optimization problems. For each convergence block, select the convergence method and the tear streams, tear variables, design specifications and/or optimization problem to be converged. You can also supply convergence parameters, such as the maximum number of iterations. The default values for the convergence parameters are established by the CONV-OPTIONS paragraph.

You can use user-generated convergence blocks with user-supplied sequences and/or automatic flowsheet analysis. When used with user-supplied sequences, user-generated convergence blocks must tear all recycle loops formed by

blocks within the sequence. (See User-Supplied Calculation Sequence, this chapter.)

When used with automatic flowsheet analysis, the user-generated convergence blocks must tear all recycle loops in the flowsheet. If you use more than one convergence block, you must also supply the convergence order.

You can enter a convergence block to converge only design specifications in the CONV-ORDER paragraph or in a user-supplied sequence, but neither is required. Design specification convergence blocks can always be placed in the calculation sequence automatically, regardless of other convergence specifications.

Use the CONVERGENCE paragraph to specify user-generated convergence blocks. Use the CONV-ORDER paragraph to specify convergence order.

The following convergence methods are available in Aspen Plus:

Method	Description	Application
WEGSTEIN	Bounded Wegstein	Tear stream, and tear variable convergence
DIRECT	Direct Substitution	Tear stream, and tear variable convergence
SECANT	Secant	Design specification convergence
BROYDEN	Broyden Quasi-Newton	Tear stream, and tear variable and/or design specification convergence
NEWTON	Newton	Tear stream, and tear variable and/or design specification convergence
COMPLEX	Complex	Optimization with inequality constraints
SQP	Sequential Quadratic Programming	Optimization with any combination of tear streams, tear variable, equality constraints and inequality constraints

WEGSTEIN Method

Input Language for WEGSTEIN

```
CONVERGENCE    cvblockid    WEGSTEIN
DESCRIPTION   "a block description - up to 64 characters in quotes"
BLOCK-OPTIONS    keyword=value
```

Optional keywords:

CONV-LEVEL TERM-LEVEL RESTART

```
TEAR    sid    [tol]    keyword = value  / ...
```

Optional keywords:

COMPS STATE TRACE

```
TEAR-VAR    keyword=value
```

Keywords:

FOR-BLOCK VAR-NAME LOWER UPPER SCALE

```
PARAM    keyword=value
```

Optional keywords:

MAXIT WAIT QMIN QMAX ACCELERATE NACCELERATE

PLOT	**plotno**	**plot-list**	*keyword=value*

Plots:

X ERROR ERR:TOL XANDERR MAXERR:TOL

Optional keywords:

TEAR COMPS STATE TEAR-VAR FOR-BLOCK PLOT-HEADING Y-SCALE X-SCALE WIDE GRID INTERPOLATE

Input Language Description for WEGSTEIN

WEGSTEIN is the classical bounded Wegstein method. It almost always converges rapidly. It is recommended for user-generated convergence blocks. WEGSTEIN can be applied to any number of streams simultaneously. You can control the Wegstein bounds and frequency of acceleration.

cvblockid ..... Convergence block ID. Cannot begin with a dollar sign.

DESCRIPTION A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the CONVERGENCE paragraph report.

BLOCK-OPTIONS Use to override the diagnostic message levels and restart option established by the DIAGNOSTICS and SIM-OPTIONS paragraphs. (See Chapter 45.)

TEAR Use to specify the tear streams to be converged by the block and optionally the tear stream convergence tolerance and convergence variables

sid..... Tear stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

tol..... Tear stream convergence tolerance. (See Note 5.) (Default=$1x10^{-4}$)

COMPS..... Component group ID. The component group should consist of a list of components to be converged in the tear stream. (See Note 5.) (Default=all components)

STATE..... State variables to be converged. (See Note 5.)

STATE=PH	Pressure and enthalpy (Default)
STATE=P	Pressure
STATE=H	Enthalpy
STATE=NONE	No state variables are converged

TRACE..... Trace component threshold. The convergence test is bypassed for components where mole fraction is less than TRACE. (Default=*tol*/100)

TEAR-VAR Use to specify tear variables to be converged by the block.

FOR-BLOCK..... Calculator block ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

VAR-NAME..... Calculator WRITE-VAR name. (See Chapter 31.)

LOWER..... Lower limit of the tear variables (Default=$-1x10^{35}$)

UPPER..... Upper limit of the tear variables (Default=$1x10^{35}$)

SCALE..... Scaling factor for the tear variables (Default=1)

PARAM Use to override default convergence parameters. You can also control the Wegstein bounds by using QMAX and QMIN and the frequency of acceleration by using ACCELERATE, NACCELERATE, and WAIT keywords.

MAXIT ..... Maximum number of flowsheet evaluations (Default=30)

WAIT ..... Number of direct substitutions before acceleration is applied (Default=1)

QMIN ..... Lower bound for *q*. (See Note 1.) (Default=-5)

QMAX ..... Upper bound for *q*. (See Note 1.) (Default=0)

ACCELERATE ..... Acceleration frequency. (See Note 1.) (Default=0)

NACCELERATE ..... Number of acceleration steps. (See Note 1.) (Default=1)

PLOT Use to generate plots and tables of the convergence history. (See Convergence Plots, this chapter.)

DIRECT Method

Input Language for DIRECT

```
CONVERGENCE    cvblockid    DIRECT
DESCRIPTION    "a block description - up to 64 characters in quotes"
BLOCK-OPTIONS  keyword=value
```

Optional keywords:

CONV-LEVEL TERM-LEVEL RESTART

```
TEAR    sid    [tol]    keyword = value    / ...
```

Optional keywords:

COMPS STATE TRACE

```
TEAR-VAR    keyword=value
```

Keywords:

FOR-BLOCK VAR-NAME

```
PARAM    MAXIT=value
PLOT     plotno    plot-list    keyword=value
```

Plots:

X ERROR ERR:TOL XANDERR MAXERR:TOL

Optional keywords:

TEAR COMPS STATE TEAR-VAR FOR-BLOCK PLOT-HEADING
Y-SCALE X-SCALE WIDE GRID INTERPOLATE

Input Language Description for DIRECT

DIRECT is the simple direct substitution method. Convergence is slow but sure. It is available for rare cases in which other methods can be unstable.

cvblockid ..... Convergence block ID. Cannot begin with a dollar sign.

DESCRIPTION A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the CONVERGENCE paragraph report.

BLOCK-OPTIONS Use to override the diagnostic message levels and restart option established by the DIAGNOSTICS and SIM-OPTIONS paragraphs. (See Chapter 45.)

TEAR Use to specify the tear streams to be converged by the block and optionally the tear stream convergence tolerance and convergence variables.

sid Tear stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

tol Tear stream convergence tolerance. (See Note 5.) (Default=$1x10^{-4}$)

COMPS Component group ID. The component group should consist of a list of components to be converged in the tear stream. (See Note 5.) (Default=all components)

STATE State variables to be converged. (See Note 5.)

STATE=PH	Pressure and enthalpy (Default)
STATE=P	Pressure
STATE=H	Enthalpy
STATE=NONE	No state variables are converged

TRACE Trace component threshold. The convergence test is bypassed for components where mole fraction is less than TRACE. (Default=*tol*/100)

TEAR-VAR Use to specify tear variables to be converged by the block.

FOR-BLOCK Calculator block ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

VAR-NAME Calculator WRITE-VAR name. (See Chapter 31.)

PARAM Use to override default convergence parameters.

MAXIT Maximum number of flowsheet evaluations (Default=30)

PLOT Use to generate plots and tables of the convergence history. (See Convergence Plots, this chapter.)

SECANT Method

Input Language for SECANT

```
CONVERGENCE    cvblockid    SECANT
DESCRIPTION    "a block description - up to 64 characters in quotes"
BLOCK-OPTIONS  keyword=value
```

Optional keywords:

CONV-LEVEL TERM-LEVEL RESTART

```
SPEC    specid    [tol]
PARAM   keyword=value
```

Optional keywords:

MAXIT STEP-SIZE MAX-STEP-SIZE XTOL BRACKET XFINAL STOP

```
PLOT    plotno    plot-list    keyword=value
```

Plots:

X ERROR ERR:TOL XANDERR MAXERR:TOL ERR-X ERR:TOL-X

Optional keywords:

SPECS PLOT-HEADING Y-SCALE X-SCALE WIDE GRID INTERPOLATE

Input Language Description for SECANT

SECANT is the secant (linear approximation) method, with higher order enhancements. SECANT can automatically switch to a bracketing/interval halving algorithm if the function is discontinuous, flat over a region, or if the function is non-monotonic. You can use SECANT to converge single design specifications. It is recommended for user-generated convergence blocks.

cvblockid ..... Convergence block ID. The ID cannot begin with a dollar sign.

DESCRIPTION A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the CONVERGENCE paragraph report.

BLOCK-OPTIONS Use to override the diagnostic message levels and restart option established by the DIAGNOSTICS and SIM-OPTIONS paragraphs. (See Chapter 45.)

SPEC Use to enter the design specification to be converged by the block and optionally the design specification tolerance. If you supply a tolerance, it overrides the value entered in the DESIGN-SPEC paragraph.

specid ..... Design specification ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

tol ..... Design specification tolerance. The specified tolerance must be a real constant. (See definition under TOL-SPEC, Chapter 30.)

PARAM Use to override default convergence parameters.

MAXIT ..... Maximum number of flowsheet evaluations (Default=30)

STEP-SIZE ..... Initial step size for the manipulated variable. The step size is defined as a fraction of the range (upper limit minus lower limit). Values specified in the DESIGN-SPEC paragraph supersede values in the CONV-OPTIONS paragraph. (Default=.01)

MAX-STEP-SIZE ..... Maximum step size for the manipulated variable. The step size is defined as a fraction of the range (upper limit minus lower limit). Values specified in the DESIGN-SPEC paragraph supersede values in the CONV-OPTIONS paragraph. (Default=1)

XTOL ..... Alternative tolerance on the manipulated variable. Iterations stop when the change in the scaled manipulated variable is less than XTOL. The variable is scaled by dividing by the absolute value of the lower limit or the upper limit, whichever is larger.
(Default=1×10^{-8})

BRACKET ..... Bracketing algorithm option:

BRACKET=YES	Switches to bracketing (and interval halving) algorithm if function does not change from one iteration to the next
BRACKET=NO	Terminates iterations if function does not change from one iteration to the next (Default)
BRACKET=CHKBNDS	Switches to bracketing (and interval halving) algorithm if function does not change from one iteration to the next, or if the secant algorithm has moved to a variable bound

XFINAL ..... Final value option. Use to specify what the final value of the manipulated variable is returned when the convergence block encounters an error.

	XFINAL=XLAST	Last value (Default)
	XFINAL=XINIT	Initial value
	XFINAL=FMIN	Value that corresponds to the best value of the function found
	XFINAL=LB	Lower bound
	XFINAL=UB	Upper bound
STOP	Specifies whether iterations should continue. Use when BRACKET=YES and the bracketing algorithm fails to find a sign change in the function.	
	STOP=NO	Iterations continue and the minimum value of the function is found
	STOP=YES	Iterations terminate (Default)
PLOT	Use to generate plots and tables of the convergence history. (See Convergence Plots, this chapter.)	

BROYDEN Method

Input Language for BROYDEN

```
CONVERGENCE   cvblockid   BROYDEN
DESCRIPTION   "a block description - up to 64 characters in quotes"
BLOCK-OPTIONS   keyword=value
```

Optional keywords:

CONV-LEVEL TERM-LEVEL RESTART

```
TEAR   sid   [tol]   keyword=value  / ...
```

Optional keywords:

COMPS STATE TRACE

```
TEAR-VAR   keyword=value
```

Keywords:

FOR-BLOCK VAR-NAME LOWER UPPER SCALE

```
SPEC   specid   [tol] / ...
PARAM   keyword=value
```

Optional keywords:

MAXIT WAIT XTOL TEAR-TOL TEAR-RATIO TEAR-MAXIT QMIN QMAX

```
STEP-SIZE   specid   stepsize  / ...
MAX-STEP-SIZE   specid   stepsize  / ...
PLOT   plotno   plot-list   keyword=value
```

Plots:

X ERROR ERR:TOL XANDERR MAXERR:TOL ERR-X ERR:TOL-X

Optional keywords:

SPECS TEAR COMPS STATE TEAR-VAR FOR-BLOCK PLOT-HEADING Y-SCALE X-SCALE WIDE GRID INTERPOLATE

Input Language Description for BROYDEN

BROYDEN is a modification of the Broyden quasi-Newton method. You can use it to converge tear streams and tear variables, two or more design specifications, or tear streams and design specifications simultaneously. BROYDEN is useful for multiple tear streams and/or design specifications when tear variables are highly interdependent, or when recycle loops and design specifications are so interrelated that nesting is impractical.

cvblockid ..... Convergence block ID. Cannot begin with a dollar sign.

DESCRIPTION A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the CONVERGENCE paragraph report.

BLOCK-OPTIONS Use to override the diagnostic message levels and restart option established by the DIAGNOSTICS and/or SIM-OPTIONS paragraphs. (See Chapter 45.)

TEAR Use to specify the tear streams converged by the block and, optionally, the tear stream convergence tolerance and convergence variables.

sid..... Tear stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

tol ..... Tear stream convergence tolerance. (See Note 5.) (Default=1×10^{-4})

COMPS ..... Component group ID. The component group should consist of a list of components to be converged in the tear stream. (See Note 5.) (Default=all components)

STATE ..... State variables to be converged. (See Note 5.)

STATE=PH	Pressure and enthalpy (Default)
STATE=P	Pressure
STATE=H	Enthalpy
STATE=NONE	No state variables are converged

TRACE ..... Trace component threshold. The convergence test is bypassed for components whose mole fraction is less than TRACE. (Default=*tol*/100)

TEAR-VAR Use to specify tear variables to be converged by the block.

FOR-BLOCK ..... Calculator block ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

VAR-NAME ..... Calculator WRITE-VAR name (See Chapter 31.)

LOWER..... Lower limit of the tear variables (Default=-1×10^{35})

UPPER..... Upper limit of the tear variables (Default=1×10^{35})

SCALE ..... Scaling factor for tear variables (Default=1)

SPEC Use to enter the design specifications to be converged by the block and, optionally, the design specification tolerance. If you supply a tolerance, it overrides the value in the DESIGN-SPEC paragraph. The specified tolerance must be a real constant. (See definition under TOL-SPEC, Chapter 30.)

specid ..... Design specification ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

tol ..... Design specification tolerance

PARAM Use to override default convergence parameters.

MAXIT ..... Maximum number of flowsheet evaluations. Each perturbation step for numerical derivatives is counted as one evaluation. (Default=30)

WAIT ..... Number of direct substitutions before acceleration is applied. Use only when tear streams are converged by the block. (Default=2)

XTOL ..... Alternative tolerance when convergence cannot be achieved because one or more variables have reached their upper or lower limits. (See Note 2.) (Default=$1x10^{-4}$)

TEAR-TOL ..... Aspen Plus initially uses Wegstein iterations to converge tear streams and tear variables to a tolerance of TEAR-TOL. Once this tolerance value is reached, Broyden iterations simultaneously converge tear streams, tear variables, and design specifications.

TEAR-RATIO ..... Aspen Plus initially uses Wegstein iterations to converge tear streams and tear variables to a tolerance of TEAR-RATIO*TOL. Once this tolerance value is reached, Broyden iterations simultaneously converge tear streams, tear variables, and design specifications.

TEAR-MAXIT ..... Maximum number of Wegstein iterations used to initially converge tear streams and tear variables, before Broyden iterations are used to simultaneously converge tear streams, tear variables, and design specifications.

QMIN ..... Lower bound on *q* during the Wegstein iterations used to initially converge tear streams and tear variables. The Wegstein iterations occur before the Broyden iterations that are used to simultaneously converge tear streams, tear variables, and design specifications. (*q* is defined in Note 1.) (Default=-5)

QMAX ..... Upper bound on *q* during the Wegstein iterations used to initially converge tear streams and tear variables. The Wegstein iterations occur before the Broyden iterations that are used to simultaneously converge tear streams, tear variables, and design specifications. (*q* is defined in Note 1.) (Default=0)

STEP-SIZE Use to enter step sizes for numerical differentiation of design specifications. Values specified in the CONVERGENCE paragraph supersede values specified in the DESIGN-SPEC paragraph.

specid ..... Design specification ID

stepsize ..... Use for the manipulated variable of the design specification when numerical derivatives are required. The step size is defined as a fraction of the range (upper limit minus lower limit). (Default=.01)

MAX-STEP-SIZE Use to enter maximum step sizes for the manipulated variables of design specifications. Use MAX-STEP-SIZE only when there are no tear streams. Values specified in the CONVERGENCE paragraph supersede values specified in the DESIGN-SPEC paragraph.

specid ..... Design specification ID

stepsize ..... Maximum step size allowed for the manipulated variable. The step size is defined as a fraction of the range (upper limit minus lower limit). (Default=1)

PLOT Use to generate plots and tables of the convergence history. (See Convergence Plots, this chapter.)

NEWTON Method

Input Language for NEWTON

```
CONVERGENCE   cvblockid   NEWTON
DESCRIPTION   "a block description - up to 64 characters in quotes"
BLOCK-OPTIONS   keyword=value
```

Optional keywords:

CONV-LEVEL TERM-LEVEL RESTART

```
TEAR   sid   [tol]   keyword=value  / ...
```

Optional keywords:

COMPS STATE TRACE

```
TEAR-VAR   keyword=value
```

Keywords:

FOR-BLOCK VAR-NAME LOWER UPPER SCALE STEP MAX-STEP

```
SPEC   specid   [tol] / ...
PARAM   keyword=value
```

Optional keywords:

MAXIT MAXPASS WAIT XTOL REINIT RED-FACTOR TEAR-TOL TEAR-RATIO TEAR-MAXIT QMIN QMAX

```
STEP-SIZE   specid   stepsize  / ...
MAX-STEP-SIZE   specid   stepsize   / ...
PLOT   plotno   plot-list   keyword=value
```

Plots:

X ERROR ERR:TOL XANDERR MAXERR:TOL ERR-X ERR:TOL-X

Optional keywords:

SPECS TEAR COMPS STATE TEAR-VAR FOR-BLOCK PLOT-HEADING Y-SCALE X-SCALE WIDE GRID INTERPOLATE

Input Language Description for NEWTON

NEWTON is an implementation of the modified Newton's method for simultaneous nonlinear equations. Derivatives are calculated only when the rate of convergence is not satisfactory. The implementation allows bounds on the variables and includes a one-dimensional search for improved stability. NEWTON is useful when the recycle loops and/or design specifications are highly interrelated but the BROYDEN method cannot converge. Since numerical derivatives are calculated frequently, use NEWTON for tear streams only when the number of components is very small or when convergence cannot be achieved by other methods.

cvblockid ..... Convergence block ID. Cannot begin with a dollar sign.

DESCRIPTION A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the CONVERGENCE paragraph report.

BLOCK-OPTIONS Use to override the diagnostic message levels and restart option established by the DIAGNOSTICS and SIM-OPTIONS paragraphs. (See Chapter 45.)

TEAR Use to specify the tear streams to be converged by the block and optionally the tear stream convergence tolerance and convergence variables.

sid Tear stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

tol Tear stream convergence tolerance. (See Note 5.) (Default=$1x10^{-4}$)

COMPS Component group ID. The component group should consist of a list of components to be converged in the tear stream. (See Note 5.) (Default=all components)

STATE State variables to be converged. (See Note 5.)

STATE=PH	Pressure and enthalpy (Default)
STATE=P	Pressure
STATE=H	Enthalpy
STATE=NONE	No state variables are converged

TRACE Trace component threshold. The convergence test is bypassed for components whose mole fraction is less than TRACE. (Default=*tol*/100)

TEAR-VAR Use to specify tear variables to be converged by the block.

FOR-BLOCK Calculator block ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

VAR-NAME Calculator WRITE-VAR name. (See Chapter 31.)

LOWER Lower limit of the tear variables (Default=$-1x10^{35}$)

UPPER Upper limit of the tear variables (Default=$1x10^{35}$)

SCALE Scaling factor for the tear variables (Default=1)

STEP Relative perturbation step (Default=0.01)

MAX-STEP Relative step limit per iteration (Default=1)

SPEC Use to enter the design specifications to be converged by the block and optionally the design specification tolerance. If tolerance is supplied here it overrides the DESIGN-SPEC value.

specid Design specification ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

tol Design specification tolerance. The specified tolerance must be a real constant. (See definition under TOL-SPEC, Chapter 30.)

PARAM Use to override default convergence parameters.

MAXIT Maximum number of Newton iterations (Default=30)

MAXPASS Maximum number of flowsheet evaluations. Each perturbation step for numerical derivatives is counted as one evaluation. (Default=100)

WAIT Number of direct substitutions before acceleration is applied. Use only when tear streams are converged by the block. (Default=2)

XTOL ..... Alternative tolerance when convergence cannot be achieved because one or more variables have reached their upper or lower limits. (See Note 2.) (Default=$1x10^{-4}$)

REINIT ..... Number of Newton iterations to use a previously calculated Jacobian (derivative) matrix before derivatives are recalculated. REINIT > 0 is used for simple (modified) Newton's method. REINIT=0 corresponds to pure Newton's method. (Default is calculated based on RED-FACTOR.)

RED-FACTOR ..... Reduction factor used in determining how many Newton iterations to use a Jacobian (derivative) matrix. If the root-mean-square of the design specification and tear stream errors divided by their respective tolerances is not reduced by a factor of RED-FACTOR, the Jacobian will be recalculated. RED-FACTOR is not used if REINIT is specified. (Default=0.2)

TEAR-TOL..... Aspen Plus initially uses Wegstein iterations to converge tear streams and tear variables to a tolerance of TEAR-TOL. Once this tolerance value is reached, Newton iterations simultaneously converge tear streams, tear variables, and design specifications.

TEAR-RATIO..... Aspen Plus initially uses Wegstein iterations to converge tear streams and tear variables to a tolerance of TEAR-RATIO*TOL. Once this tolerance value is reached, Newton iterations simultaneously converge tear streams, tear variables, and design specifications.

TEAR-MAXIT ..... Maximum number of Wegstein iterations used to initially converge tear streams and tear variables, before Newton iterations are used to simultaneously converge tear streams, tear variables, and design specifications.

QMIN ..... Lower bound on *q* during the Wegstein iterations used to initially converge tear streams and tear variables. The Wegstein iterations occur before the Newton iterations that are used to simultaneously converge tear streams, tear variables, and design specifications. (*q* is defined in Note 1.) (Default=−5)

QMAX..... Upper bound on *q* during the Wegstein iterations used to initially converge tear streams and tear variables. The Wegstein iterations occur before the Newton iterations that are used to simultaneously converge tear streams, tear variables, and design specifications. (*q* is defined in Note 1.) (Default=0)

STEP-SIZE

Use to enter step sizes for numerical differentiation of design specifications. Values specified in the CONVERGENCE paragraph supersede values specified in the DESIGN-SPEC paragraph.

specid ..... Design specification ID

stepsize ..... Step size to be used for the manipulated variable of the design specification when numerical derivatives are required. The step size is defined as a fraction of the range (upper limit minus lower limit). (Default=0.01)

MAX-STEP-SIZE

Use to enter maximum step sizes for the manipulated variables of design specifications. Values specified in the CONVERGENCE paragraph supersede values specified in the DESIGN-SPEC paragraph.

specid ..... Design specification ID

stepsize ..... Maximum step size allowed for the manipulated variable. The step size is defined as a fraction of the range (upper limit minus lower limit). (Default=1)

PLOT Use to generate plots and tables of the convergence history. (See Convergence Plots, this chapter.)

COMPLEX Method

Input Language for COMPLEX

```
CONVERGENCE    cvblockid    COMPLEX
DESCRIPTION   "a block description - up to 64 characters in quotes"
BLOCK-OPTIONS    keyword=value
```

Optional keywords:

CONV-LEVEL TERM-LEVEL RESTART

```
OPTIMIZE    optid
PARAM    keyword=value
```

Optional keywords:

MAXIT NPOINT EXP-FACTOR CONTR-FACTOR REFL-FACTOR RTOL ATOL

```
STEP-SIZE    varyno    stepsize  /  ...
```

Input Language Description for COMPLEX

COMPLEX is the Complex optimization method. You can use it to converge optimization problems with bounds on the manipulated variables and optionally inequality constraints. COMPLEX is a direct search method. It does not require numerical derivatives. It can be useful for simple problems without recycle loops or equality constraints (design specifications).

cvblockid ..... Convergence block ID. Cannot begin with a dollar sign.

DESCRIPTION A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the CONVERGENCE paragraph report.

BLOCK-OPTIONS Use to override the diagnostic message levels and restart option established by the DIAGNOSTICS and SIM-OPTIONS paragraphs. (See Chapter 45.)

OPTIMIZE Use to specify the optimization problem to be converged.

optid ..... Optimization ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

PARAM Use to override default convergence parameters.

MAXIT..... Maximum number of flowsheet evaluations (Default=60)

NPOINT..... Maximum number of points in the simplex. Must be between number of variables + 2, and 2*number of variables. (Default=number of variables + 2)

EXP-FACTOR ..... Factor used to expand the size of the simplex (Default=1.3)

CONTR-FACTOR..... Factor used to contract the size of the simplex (Default=0.5)

REFL-FACTOR..... Factor used to "reflect" variables when bounds or inequality constraints are encountered (Default=0.1)

RTOL..... Relative convergence tolerance (Default=$1x10^{-4}$)

ATOL..... Absolute convergence tolerance (Default=$1x10^{-4}$)

STEP-SIZE

Use to specify the range used for generating random points in the initial simplex. If the initial variable value is close to the optimum, a range less than one helps the problem converge faster.

varyno ..... Decision variable number

stepsize ..... Step size used for generating random points in the initial simplex. The step size is defined as a fraction of the range (upper limit minus lower limit). (Default=1.0)

SQP Method

Input Language for SQP

```
CONVERGENCE   cvblockid   SQP
DESCRIPTION   "a block description - up to 64 characters in quotes"'
BLOCK-OPTIONS   keyword=value
```

Optional keywords:

CONV-LEVEL TERM-LEVEL RESTART

```
OPTIMIZE   optid
TEAR   sid   [tol]   keyword = value  / ...
```

Optional keywords:

COMPS STATE TRACE

```
TEAR-VAR   keyword=value
```

Keywords:

FOR-BLOCK VAR-NAME LOWER UPPER SCALE STEP MAX-STEP

```
PARAM   keyword=value
```

Optional keywords:

MAXIT MAXPASS WAIT TOL QMIN QMAX MAXLSPASS NLIMIT PRINT-PLOT STEP-OPT STEP-DIR OPT-METHOD DERIVATIVE EST-STEP
CONST-ITER DERIV-SWITCH STEP-PRES STEP-ENTH STEP-FLOW STEP-HEAT VAR-MIN CONV-TEST

```
STEP-SIZE   varyno   stepsize  / ...
SCALE   varyno   scale  / ...
MAX-STEP-SIZE   varyno   stepsize  / ...
```

Input Language Description for SQP

SQP is the state-of-the-art sequential quadratic programming method for flowsheet optimization. You can use SQP for simultaneous convergence of

optimization problems with constraints (equality or inequality), tear variables, and/or tear streams. The algorithm generally follows an infeasible path (constraints, tear streams, and tear variables are converged simultaneously with the optimization problem), but can be adjusted to follow a feasible path (converging the tear streams and tear variables at each iteration of the optimization). Use SQP for system-generated optimization convergence blocks. It is recommended for user-generated convergence blocks.

cvblockid ..... Convergence block ID. Cannot begin with a dollar sign.

DESCRIPTION A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the CONVERGENCE paragraph report.

BLOCK-OPTIONS Use to override the diagnostic message levels and restart option established by the DIAGNOSTICS and SIM-OPTIONS paragraphs. (See Chapter 45.)

OPTIMIZE Use to specify the optimization problem to be converged.

optid ..... Optimization ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

TEAR Use to specify the tear streams converged by the block and optionally the tear stream convergence tolerance and convergence variables.

sid..... Tear stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

tol ..... Tear stream convergence tolerance. (See Note 5.) (Default=$1x10^{-4}$)

COMPS ..... Component group ID. The component group should consist of a list of components to be converged in the tear stream. (See Note 5.) (Default=all components)

STATE ..... State variables to be converged. (See Note 5.)

STATE=PH	Pressure and enthalpy (Default)
STATE=P	Pressure
STATE=H	Enthalpy
STATE=NONE	No state variables are converged

TRACE ..... Trace component threshold. The convergence test is bypassed for components whose mole fraction is less than TRACE. (Default=*tol*/100)

TEAR-VAR Use to specify tear variables to be converged by the block.

FOR-BLOCK ..... Calculator block ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

VAR-NAME ..... Calculator WRITE-VAR name. (See Chapter 31.)

LOWER..... Lower limit of the tear variables (Default=$-1x10^{35}$)

UPPER..... Upper limit of the tear variables (Default=$1x10^{35}$)

SCALE ..... Scaling factor for the tear variables (Default=1)

STEP ..... Relative perturbation step (Default=0.01)

MAX-STEP ..... Relative step limit per iteration (Default=1)

PARAM Use to override default convergence parameters.

MAXIT..... Maximum number of sequential quadratic programming iterations (Default=30)

MAXPASS	Maximum number of flowsheet evaluations. Each perturbation step for numerical derivatives is counted as one evaluation. (Default=99999)	
WAIT	Number of direct substitutions before acceleration is applied. Use only when tear streams are converged by the block. (Default=2)	
TOL	Convergence tolerance (Default=$1x10^{-3}$)	
QMIN	Lower bound on *q* for Wegstein iterations to converge tear streams. (See Note 3.) *q* is defined in Note 1. (Default=-5)	
QMAX	Upper bound on *q* for Wegstein iterations to converge tear streams. (See Note 3.) *q* is defined in Note 1. (Default=0)	
MAXLSPASS	Number of iterations to take toward converging the tear streams at each iteration of the optimization. (See Note 3.) (Default=3)	
NLIMIT	Number of iterations to enforce maximum steps on the manipulated variables (Default=3)	
PRINT-PLOT	**PRINT-PLOT=YES**	Produces print-plots of the manipulated variable, objective function, and Lagrangian (penalty) function and constraint values versus iteration number (Default)
	PRINT-PLOT=NO	Does not produce print-plots
STEP-OPT	Specifies how perturbation step size (given in the STEP-SIZE sentence) is interpreted:	
	STEP-OPT=RANGE	Perturbation step = step size * (upper limit – lower limit) (Default)
	STEP-OPT=VARIABLE	Perturbation step=step size * variable value
	STEP-OPT=VALUE	Perturbation step=step size
STEP-DIR	Direction to perturb variables:	
	STEP-DIR=NEGATIVE	Negative direction (Default)
	STEP-DIR=POSITIVE	Positive direction
OPT-METHOD	Optimization method:	
	OPT-METHOD=SQP	Sequential quadratic programming algorithm (Default)
	OPT-METHOD=SLP	Sequential linear programming algorithm
DERIVATIVE	Specifies whether to use central or forward difference for derivative calculations: FORWARD or CENTRAL (Default=FORWARD)	
EST-STEP	Specifies whether to perform automatic step-size determination: YES or NO (Default=NO)	
CONST-ITER	Number of additional iterations when constraints are not satisfied after convergence test is satisfied (Default=2)	
DERIV-SWITCH	Specifies whether to switch to central difference on convergence failure: YES or NO (Default=NO)	
STEP-PRES	Relative perturbation step for pressure tear variables (Default=0.01)	
STEP-ENTH	Relative perturbation step for enthalpy tear variables (Default=0.01)	
STEP-FLOW	Relative perturbation step for flow tear variables (Default=0.01)	
STEP-HEAT	Relative perturbation step for heat tear variables (Default=0.01)	

VAR-MIN ..... Specifies minimum variable value for step size calculation when STEP-OPT=VARIABLE (Default=$1x10^{-4}$)

CONV-TEST ..... Convergence test options:

CONV-TEST=KKT	Kuhn-Tucker using Hessian (Default)
CONV-TEST=KKT1	Kuhn-Tucker using first order conditions
CONV-TEST=RG	Reduced gradient
CONV-TEST=RGRD	Reduced gradient with step constraints

STEP-SIZE

Use to enter decision variable step sizes for numerical differentiation. Values specified in the CONVERGENCE paragraph supersede values specified in the OPTIMIZATION paragraph.

varyno ..... Decision variable number

stepsize ..... Step size to be used for the decision variable when numerical derivatives are required. The definition of step size depends on the option selected for STEP-OPT in the PARAM sentence. (Default=.01)

SCALE

Use to enter scale factors for the decision variables. (See Note 4.)

varyno ..... Decision variable number

scale ..... Scale factor (Default=1)

MAX-STEP-SIZE

Use to specify the maximum step sizes for the decision variables. The maximum step size is enforced for the first NLIMIT steps. Values specified in the CONVERGENCE paragraph supersede values specified in the OPTIMIZATION paragraph.

varyno ..... Decision variable number

stepsize ..... Maximum step size allowed for the decision variable. The step size is defined as a fraction of the range (upper limit minus lower limit). (Default=1)

CONV-ORDER Paragraph

Input Language for CONV-ORDER

```
CONV-ORDER    cvblockid-list
```

Input Language Description for CONV-ORDER

Use the CONV-ORDER paragraph to specify the calculation order of user-defined convergence blocks. You can enter the convergence blocks in the order in which you prefer the nested loops to be solved. The CONV-ORDER paragraph is non-hierarchical but you can specify convergence blocks inside hierarchies.

cvblockid-list ..... Convergence block ID list. The first convergence block entered is converged first and is nested most deeply. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

Convergence Plots

Input Language for PLOT

```
PLOT    plotno    plot-list    keyword=value
```

Plots:

X ERROR ERR:TOL XANDERR MAXERR:TOL ERR-X ERR:TOL-X

Optional keywords:

SPECS TEAR COMPS STATE TEAR-VAR FOR-BLOCK PLOT-HEADING Y-SCALE X-SCALE WIDE GRID INTERPOLATE

Input Language Description for PLOT

You can use the PLOT sentence in WEGSTEIN, DIRECT, SECANT, BROYDEN, and NEWTON convergence block paragraphs to generate plots and/or convergence history tables. You can also generate plots in SQP optimization convergence blocks, using the PRINT-PLOT keyword in the PARAM sentence.

PLOT Use in convergence block paragraphs to generate plots and tables of iteration histories. For all plots except MAXERR:TOL, the variables and errors to be plotted are selected using SPECS, TEAR, COMPS, and STATE.

plotno ..... Plot number

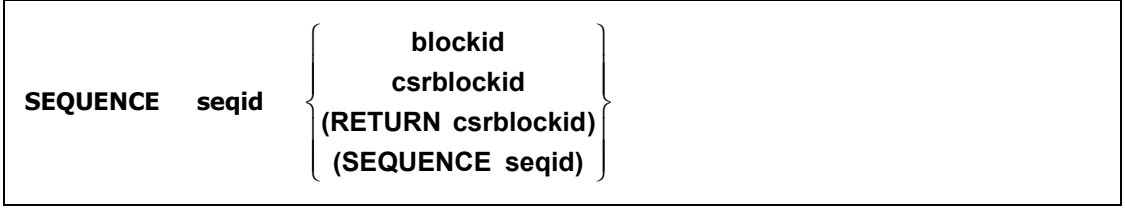
plot-list ..... List of convergence plots to be generated. If you enter a PLOT sentence but do not specify *plot-list*, MAXERR:TOL will be plotted.

X	Plots convergence variables versus iteration number
ERROR	Plots errors versus iteration number
ERR:TOL	Plots error/tolerance versus iteration number
XANDERR	Plots convergence variables and errors versus iteration number
MAXERR:TOL	Plots maximum error/tolerance versus iteration number

	ERR-X	Plots design-spec errors versus varied variables
	ERR:TOL-X	Plots design-spec errors/tolerance versus varied variables
SPECS		List of IDs for the design specifications to be plotted. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.
TEAR		List of stream IDs for the tear streams to be plotted. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.
COMPS		List of component IDs and component group IDs. Use to control the plotting of tear stream component variables. (Default=all components)
STATE		Use to control the plotting of tear stream state variables:
	STATE=PH	Plots pressure and enthalpy (Default)
	STATE=P	Plots pressure
	STATE=H	Plots enthalpy
	STATE=NONE	Does not plot state variables
TEAR-VAR		List of Calculator WRITE-VAR names to be plotted. (See Chapter 31.) Can be hierarchical; see Chapter 9 for naming conventions and restrictions.
FOR-BLOCK		List of Calculator block IDs to be plotted. (See Chapter 31.) Can be hierarchical; see Chapter 9 for naming conventions and restrictions.
PLOT-HEADING		Heading up to 64 characters enclosed in quotes printed at top of each plot and table. (Different defaults for each type of table and plot are built in.)
Y-SCALE	**Y-SCALE=STANDARD**	Uses linear scale on vertical axis of plots (Default)
	Y-SCALE=INVERSE	Uses inverse scale on vertical axis of plots
	Y-SCALE=LOG	Uses logarithmic scale on vertical axis of plots
X-SCALE	**X-SCALE=STANDARD**	Uses linear scale on horizontal axis of plots (Default)
	X-SCALE=INVERSE	Uses inverse scale on horizontal axis of plots
WIDE, GRID, INTERPOLATE		Plot options. Use to override defaults established by PLOT-OPTIONS paragraph. (See Chapter 46.)

User-Supplied Calculation Sequence

Input Language for SEQUENCE



Input Language Description for SEQUENCE

Use the SEQUENCE paragraph to specify the calculation order for all or part of the flowsheet. A sequence specification consists of block IDs, convergence or sensitivity block IDs (the beginning of a loop), and convergence or sensitivity block returns (the end of a loop) in order of execution. User-supplied sequences can be nested, that is, one user-supplied sequence can refer to another user-supplied sequence. The SEQUENCE paragraph is hierarchical and you can also specify blocks inside hierarchies.

seqid	Sequence ID
blockid	Unit operation, Calculator, transfer, balance, or pressure relief block ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.
csrblockid	Convergence, sensitivity, or regression block ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.
(RETURN csrblockid)	Indicates that control is returned to convergence, sensitivity, or regression block *csrblockid* until the convergence loop or regression loop is converged or fails to converge, or the sensitivity is completed. The block *csrblockid* must have already appeared in the sequence. You must enter the parentheses as shown. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.
(SEQUENCE seqid)	Indicates that sequence *seqid* is to be executed at this point. You must enter the parentheses as shown. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

Notes

1 When the bounded Wegstein method is used, an acceleration parameter *q* is calculated for each tear stream variable as follows:

$$q = \frac{s}{s-1}$$

$$s = \frac{G(X_k) - G(X_{k-1})}{X_k - X_{k-1}}$$

Where *X* is an estimate of the tear stream variable, *G*(*X*) is the resulting calculated value of the variable, and *k* is the iteration number. The new estimate calculated by Wegstein is:

$$X_{k+1} = X_k + (1-q)\,G(X_k)$$

The following table shows the effect of *q* on convergence:

q	Convergence
$q < 0$	Acceleration
$q = 0$	Direct substitution
$0 < q < 1$	Damping

Because oscillation or divergence can occur if q is unbounded, limits are set on q. The default for QMAX, the upper bound, is 0. The default for QMIN, the lower bound, is -5. For most flowsheets, these limits work well and do not need to be changed.

Normally a QMAX of 0 should be used. If iterations move the variables slowly toward convergence, smaller values of QMIN (for example, -25 or -50) may give better results. If oscillation occurs with direct substitution, values of QMIN and QMAX between 0 and 1 may help.

You can control the Wegstein method by specifying:

- Upper and lower limits for *q* (QMAX and QMIN)
- The number of direct substitution iterations before the first acceleration (WAIT)
- The number of direct substitution iterations between acceleration iterations (ACCELERATE)
- The number of consecutive acceleration iterations (NACCELERATE)

2 When the NEWTON or BROYDEN methods are used to converge design specifications and one or more manipulated variables have reached their lower or upper limits, Aspen Plus finds a solution which minimizes the sum-of-squares of design specification and tear stream errors divided by their respective tolerances. Iterations stop when the root-mean-square of the changes in the scaled manipulated variables is less than XTOL. Each manipulated variable is scaled by dividing by the absolute value of the lower limit or of the upper limit, whichever is larger.

3 When you use the SQP method to converge tear streams and optimization problems simultaneously, the algorithm is a hybrid of an infeasible path method (where the tear streams are not converged at each iteration but are converged at the optimum) and a feasible path method (where the tear streams are converged at each iteration of the optimization). You can control the degree to which the tear streams are converged by specifying the number of iterations to take toward converging the tear streams (MAXLSPASS) and upper and lower limits for *q* for the Wegstein iterations (QMAX and QMIN).

4 For the SQP method, decision variables are automatically scaled by dividing by the maximum of the upper and lower bound on the variable. Scale factors entered in the SCALE statement are then used to multiply the variable (and thus divide the corresponding element of the gradient). The default scaling procedure is usually sufficient. Scale factors should be used when the effect of a decision variable on the objective function is under emphasized.

5 A tear stream is converged when

$$-tol \le \frac{X_{calculated} - X_{assumed}}{X_{assumed}} \le tol$$

for all stream convergence variables. This convergence test is bypassed for components whose mole fraction is less than TRACE. The default for TRACE is *tol*/100. The default convergence variables are the component mole flows for all components, pressure, and enthalpy.

You can use COMPS to select convergence variables when some components are known to have zero or constant flow rates. You can use STATE when pressure is known to be constant, or enthalpy is not calculated (that is, mass balance only simulations). COMPS and STATE are intended primarily for use with the matrix convergence methods (BROYDEN, NEWTON, and SQP) in order to reduce the matrix size and the number of numerical derivative perturbations.

38 Fitting a Simulation Model to Data

This chapter describes the input language for fitting a simulation model to data. Two types of data can be fit: point data and profile data.

Use the DATA-SET paragraph to define and enter point data. Examples of point data are:

- Scalar variables from one or more steady-state experiments or operating points.
- Initial and final product conditions of a batch reactor.
- Feed and product conditions of a plug flow reactor.

Use the PROFILE-DATA paragraph to define and enter profile data. Examples of profile data are:

- Time series data for a batch reactor.
- Measurements along the length of a plug flow reactor.

Use the REGRESSION paragraph to specify regression cases and convergence parameters.

DATA-SET Paragraph

Input Language for DATA-SET

```
DATA-SET    datasetid
DESCRIPTION    "a data-fit description - up to 64 characters in quotes"
DEFINE    fvar    vartype    keyword=value
INPUT    var-list
RESULT    var-list
USE    datatype    value-list  /  . . .
```

Input Language Description for DATA-SET

datasetid..... DATA-SET paragraph ID

DESCRIPTION A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the data-fit report.

DEFINE Use to access a flowsheet variable and equivalence it to the DATA-SET variable *fvar*. There must be at least one DEFINE sentence in a DATA-SET paragraph. The DEFINE statements must appear in the same order as the corresponding data in the USE statement. See Chapters 29 and 30 for a complete description of the DEFINE sentence.

INPUT, RESULT Use to establish which DATA-SET variables are input variables and which are result variables. Enter feed stream variables and block input parameters in the INPUT sentence, to classify them as input variables. Enter calculated variables in the RESULT sentence to classify them as results.

var-list..... List of DATA-SET variables

USE Use to enter standard deviation and measurement data for the DATA-SET variables.

datatype ..... Use STD-DEV to indicate that the following *value-list* values are standard deviation values. Use DATA to indicate that the following *value-list* values are measurement values. The first data type must always be STD-DEV. You can enter subsequent values for standard deviations to override the initial values. In this case, the new standard deviation values apply only to the measurements that follow.

value-list ..... Standard deviation or measurement values for the data point. There must be one value for each DEFINE statement. The order of the values must correspond to the order of the DEFINE statements. Missing measurement values are indicated by replacing the appropriately positioned value with an asterisk (*). Negative standard deviation values represent percentages of the measurement values.

PROFILE-DATA Paragraph

Input Language for PROFILE-DATA

```
PROFILE-DATA    profileid
DESCRIPTION    "a data-fit description - up to 64 characters in quotes"
PARAM    keyword=value
```

Keywords:

BLOCK-TYPE BLOCK TEMP PRES UNITS

```
DEFINE  ZZTEMP  BLOCK-VAR  BLOCK=blockid  SENTENCE=PARAM  &
      VARIABLE=TEMP
DEFINE  ZZPRES  BLOCK-VAR  BLOCK=blockid  SENTENCE=PARAM  &
      VARIABLE=PRES
VECTOR-DEF  farray  BLOCK-VEC  BLOCK=blockid  SENTENCE=sentname  &
      VARIABLE=varname  [ID2=id2]
USE  datatype  value-list  / . . .
basis-FLOW  cid  value  / . . .
```

Input Language Description for PROFILE-DATA

profileid PROFILE-DATA paragraph ID

DESCRIPTION A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the data-fit report.

PARAM Use to enter the block type, block ID, inlet temperature, and inlet pressure. You can also enter units for the reactor profile variable.

BLOCK-TYPE ..... Specifies model to be used to fit measured profiles:

BLOCK-TYPE=RBATCH	Rigorous batch or semibatch reactor (Default)
BLOCK-TYPE=RPLUG	Rigorous plug flow reactor

BLOCK..... ID of block where profiles have been measured. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

TEMP..... Reactor inlet temperature to replace the base case value for this data set. If you use TEMP, the DEFINE ZZTEMP sentence must be present. TEMP is not allowed when BLOCK-TYPE=RPLUG.

PRES..... Reactor inlet pressure (if PRES>0), or pressure drop (if PRES≤0), to replace the base case value for this data set. If you use PRES, the DEFINE ZZPRES sentence must be present.

UNITS..... Units for reactor profile variable (length or time)

DEFINE ZZTEMP, DEFINE ZZPRES Use to access the reactor temperature and pressure. You can use DEFINE ZZTEMP only when BLOCK-TYPE=RBATCH.

blockid..... Block ID. Defined in the BLOCK keyword, where profiles have been measured. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

VECTOR-DEF

Use to access a flowsheet profile and equivalence it to the PROFILE-DATA array, *farray*. There must be at least one VECTOR-DEF sentence in a PROFILE-DATA paragraph. The VECTOR-DEF statements must appear in the same order as the corresponding data in the USE statement. See Chapters 29 and 30 for further information on the use of VECTOR-DEF.

farray..... FORTRAN array name limited to five characters. Aspen Plus will explicitly declare *farray* as double precision or integer, based on the type of the accessed variable.

blockid..... Block ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

sentname..... Sentence name. (See Accessing Variables in RBATCH and RPLUG, this chapter.)

varname ..... Variable name. (See Accessing Variables in RBATCH and RPLUG, this chapter.)

id2 ..... Variable ID used to uniquely identify the accessed variable, when the variable name alone is insufficient. (See Accessing Variables in RBATCH and RPLUG, this chapter.)

USE

Use to enter standard deviation and measurement data for the PROFILE-DATA variables. The number and location of measurement points must coincide with those defined on the reactor REGR-PARAM and REGR-POINTS sentences. (See Chapter 19.) The location values in the USE sentence are in units specified in the PARAM sentence, while the REGR-POINTS location values are always in SI units.

datatype ..... Data type. The first datatype must always be STD-DEV:

STD-DEV	Indicates the following *value-list* values are standard deviation values. Subsequent values for standard deviations can be entered to override the initial values. In this case, the new standard deviation values apply only to measurements that follow.
DATA	Indicates the following *value-list* values are measurement values

value-list ..... Standard deviation or measurement values for the data point. The first value must be the measurement location value (length or time). It is followed by standard deviation or measurement values. There must be one value for each VECTOR-DEF statement. The order of values must correspond to the order of VECTOR-DEF statements. You can indicate missing measurement values by replacing the appropriately positioned value with an asterisk (*). Negative standard deviation values represent percentages of the measurement values.

basis-FLOW

Use to enter component flows on a MOLE, MASS, or STDVOL basis, to replace the base case values for this data-set.

cid..... Component ID

value..... Component mole, mass, or standard-liquid-volume flow rate

Accessing Variables in RBATCH and RPLUG

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for an RBATCH or RPLUG block.

Block Input

Using RBATCH block type:

Sentence	Variables	ID2
REGR-C-PROF	PARTIAL-PRES, MOLECONC-L, MASSCONC-L, MOLEFRAC-L, MASSFRAC-L, MOLECONC-V, MOLEFRAC-V	cid
REGR-LS-PROF	MASSCONC-LS	cid
REGR-PROF	TEMPERATURE, PRESSURE, DUTY, CUM-DUTY, VENT-MOLFLOW, VENT-VOLFLOW	—
REGR-RP-PROF	REACTOR-PROP	pid (Property set ID)
REGR-AP-PROF	ACCUM-PROP	pid (Property set ID)
REGR-VP-PROF	VENT-PROP	pid (Property set ID)

Using RPLUG block type:

Sentence	Variables	ID2
REGR-C-PROF	PARTIAL-PRES, MOLECONC-L, MASSCONC-L, MOLEFRAC-L, MASSFRAC-L, MOLECONC-V, MOLEFRAC-V	cid
REGR-LS-PROF	MASSCONC-LS	cid
REGR-PROF	TEMPERATURE, PRESSURE	—

REGRESSION Paragraph

Input Language for REGRESSION

```
REGRESSION    rblockid
DESCRIPTION   "a data-fit description - up to 64 characters in quotes"
DATA    setid    weight  / . . .
VARY    vartype    keyword=value
LIMITS    lower    upper
BLOCK-OPTION    SIM-LEVEL=value
ALGORITHM    keyword=value
```

Keywords:

BOUND-FAC MAX-ITER COVAR-REQ INIRIN AFCTOL RFCTOL XCTOL XFTOL TUNER1 TUNER2 TUNER3 INIT-STEP DECFAC INCFAC RDFCMN RDFCMX FUZZ DFAC MXPASS PERT-FAC

Input Language Description for REGRESSION

rblockid..... Regression block ID

DESCRIPTION A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the data-fit report.

DATA Use to specify data sets and data set weighting to be used in the regression case.

setid ..... DATA-SET or PROFILE-DATA paragraph ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

weight ..... Relative weight of the data (Default=1)

VARY Use to identify parameters to estimate. Only block input or process feed stream variables can be estimated. The estimated block or stream variable must either be a variable that you specify in a BLOCK or STREAM paragraph, or it must have a default value. See Chapters 29 and 30 for a complete description of the VARY sentence.

LIMITS Use to specify limits for the estimated parameter.

lower ..... Lower bound of varied variable

upper ..... Upper bound of varied variable

BLOCK-OPTION Use to override the diagnostic message levels established by the DIAGNOSTIC paragraph. (See Chapter 45.)

ALGORITHM Use to enter optional convergence and tuning parameters.

BOUND-FAC ..... Use in computing the lower and upper bounds for the reconciled input variables. The bounds are calculated from the absolute value of the standard deviation for the measurement (S), and the BOUND-FACTOR value (B) as follows:

UpperBound=MeasuredValue + B*S
LowerBound=MeasuredValue – B*S (Default=10)

MAX-ITER ..... Maximum number of data-fit algorithm iterations (Default=50)

COVAR-REQ ..... **COVAR-REQ=YES** Calculates covariance matrix (Default)

COVAR-REQ=NO Does not calculate covariance matrix

INIRIN Specifies whether the reconciled INPUT variables are to be initialized to their base-case values or to measurements:

1	Measurements
0	Base-case (Default)

AFCTOL Sum-of-squares objective function tolerance. Data-fit will be considered converged if objective functions ≤ AFCTOL. (Default=0.01)

RFCTOL Relative function convergence tolerance (Default=$2x10^{-3}$)

XCTOL X convergence tolerance. Data-fit is considered converged if the scaled distance of the current X, from the optimal X, is less than XCTOL. (Default=$2x10^{-3}$)

XFTOL Data-fit returns with suboptimal solution, if a step of scaled length of at most XFTOL is tried but not accepted. (Default=$1x10^{-10}$)

TUNER1 Parameter used to check for false convergence. This parameter is also used to select convergence algorithm for the current trust region. (Default=0.1)

TUNER2 Step-size control parameter. For a step to be accepted, the actual function reduction must be more than TUNER2 times its predicted value. (Default=$1x10^{-4}$)

TUNER3 Trust region adjustment factor. The trust region radius is increased if the actual decrease in objective function is at least TUNER3*inner_product of the step and the gradient. (Default=0.75)

INIT-STEP Factor determining the initial step-size (Default=1.0)

DECFAC Factor by which the trust region radius is reduced, if the current X lead to errors in function or Jacobian evaluation (Default=0.5)

INCFAC Minimum factor by which the trust region radius can be increased (Default=2.0)

RDFCMN Minimum factor by which the trust region radius can be reduced (Default=0.1)

RDFCMX Maximum factor by which the trust region radius can be increased at one time (Default=4.0)

FUZZ Parameter for determining when to switch the convergence method used for the trust region (Default=1.5)

DFAC Tuning factor associated with the adaptive scaling strategy used in the algorithm (Default=0.6)

MXPASS Maximum number of flowsheet passes allowed in a data-fit run. MXPASS includes flowsheet passes for the initial base case, passes required to compute the residuals, and passes required to compute the Jacobian matrix through perturbation. (Default=1000)

PERT-FAC Relative perturbation size for Jacobian evaluation. Perturbation step-size variable X is PERT-FACTOR*absolute value of X. (Default=$5x10^{-3}$)

39 Pressure Relief

This chapter describes the input language for modeling pressure relief systems and simulating vessels undergoing de-pressurization.

The PRES-RELIEF block can be used to model dynamic or steady-state situations. Depending on the scenario chosen, different specifications are required. The following scenarios are allowed:

Scenario	Description
FIRE	Dynamic scenario with vessel exposed to external fire
HEAT-INPUT	Dynamic scenario with fixed or variable heat flux into vessel
FLOW-SPEC	Steady-state valve rating scenario with piping
VALVE-RATING	Steady-state simple valve rating scenario with no piping

PRES-RELIEF Block

Input Language for PRES-RELIEF

```
PRES-RELIEF    pblockid
PROPERTIES     keyword=value
```

Optional keywords:

OPSETNAME HENRY-COMPS CHEMISTRY TRUE-COMPS FREE-WATER SOLU-WATER

```
BLOCK-OPTIONS    keyword=value
```

Optional keywords:

SIM-LEVEL PROP-LEVEL TERM-LEVEL RESTART

```
PARAM    keyword=value
```

Keywords:

SCENARIO CAPACITY NPHASE DISENGAGEMENT VFRAC DISCHARGE-PR MAXIT TOL REACTION VES-BASIS STRM-BASIS basis-FLOW MAX-TIME PRINT-TIME ADD-POINTS MAX-NPOINT OPEN-TIME VENT-NPHASE VENT-PHASE

```
REFERENCE    STREAM=sid
VESSEL-FRAC    cid    frac  /  ...
STREAM-FRAC    cid    frac  /  ...
VESSEL    keyword=value
```

Keywords:

VES-TYPE MAWP MAWP-TEMP HEADS HEAD-AREA HEAD-VOL DIAMETER LENGTH MOUNT JACKET-VOL VES-VOLUME VES-AREA VES-NECK-DIA VES-NECK-DIR VES-NECK-LEN VES-NECK-CON VES-NECK-RUF REDUCER-K EXPANDER-K DEAD-VOL

```
CONDITIONS    keyword=value
```

Keywords:

FILLAGE PAD-COMP VES-TEMP VES-PRES VES-VFRAC VES-TFROM VES-PFROM VES-VFFROM STRM-TEMP STRM-PRES STRM-VFRAC STRM-TFROM STRM-PFROM STRM-VFFROM

```
REACTIONS    REACID=reacid-list
FIRE    keyword=value
```

Keywords:

STANDARD ELEVATION DRAINAGE WATER-SPRAY INSULATION PORTABLE CREDIT-FACT EXTRA-AREA FIRE-TIME INS-CREDIT DR-AND-FF LIQ-LEVEL

```
DUTY-PROF    time    duty  /  ...
HEAT-INPUT    keyword=value
```

Keywords:

TEMP U AREA DUTY

RELIEF-DEV *keyword=value*

Keywords:

DEVICE PSV-SERVICE PSV-THROAT PSV-IN-DIAM PSV-OUT-DIAM PSV-CD PSV-OVER-PR PSV-SETPOINT PSV-OPEN PSV-CLOSE PSD-DIAM PSD-CD PSD-LD PSD-SETPOINT ERV-DIAM ERV-SETPOINT ERV-OVER-PR COMB-COEF N-INLET-SECT N-TAIL-SECT

INLET-PIPE secno *keyword=value*

Keywords:

ACTUAL-DIAM LENGTH CONNECTIONS

Optional keywords:

ELEVATION ELBOWS STRAIGHT-TEE BRANCHED-TEE GATE-VALVES BUTTERFLY-VA VALVE-AREA VALVE-COEFF CONTROL-CV MISC-L-D TAMBIN TAMBOUT U REDUCER-K EXPANDER-K ROUGHNESS

TAIL-PIPE secno *keyword=value*

Keywords:

ACTUAL-DIAM LENGTH CONNECTIONS

Optional keywords:

ELEVATION ELBOWS STRAIGHT-TEE BRANCHED-TEE GATE-VALVES BUTTERFLY-VA VALVE-AREA VALVE-COEFF CONTROL-CV MISC-L-D TAMBIN TAMBOUT U REDUCER-K EXPANDER-K ROUGHNESS

STOP stopno location variable value from *keyword=value*

Locations:

VESSEL ACCUMULATOR VENT

Variables:

TIME MASS-FRAC MOLE-FRAC CONVERSION MOLES MASS TEMP MOLE-FLOW MASS-FLOW VFRAC PRES

Keywords:

COMP SUBSTREAM

RULES *keyword=value*

Keywords:

IN-MAXFAC TAIL-ALLFAC RESPOND EQP-MAXFAC EQP-MAXPRE SPCHANGE

REPORT reportopt-list

Reportopts:

NOREPORT NEWPAGE NOINPUT NORESULTS

CONVERGENCE keyword=value

Keywords:

SFLASH-MAXIT SFLASH-TOL BUBBLY-C0 CHURN-C0 VALVE-SFLASH CVT-SFLASH VAL-SIMPSON CVT-SIMPSON INLET-TABLE INLET-NT INLET-NP TAIL-TABLE TAIL-NT TAIL-NP DEVICE-ONLY PRES-TOL FLOW-TOL FRIC-DOWNHILL FRIC-HORIZ FRIC-INCL FRIC-VERTICA HOLDUP-DOWNH HOLDUP-HORIZ HOLDUP-INCL HOLDUP-VERTI STOP-CYCLING MAX-NCYCLE CYCLE-TIME ATMOS-PRES BA-H0 BA-HMXUSR BA-RINTOL BA-CORR-METH VA-H0 VA-HMXUSR VA-RINTOL VA-CORR-METH CV-H0 CV-HMXUSR CV-RINTOL CV-CORR-METH IN-H0 IN-HMXUSR IN-RINTOL IN-CORR-METH TA-H0 TA-HMXUSR TA-RINTOL TA-CORR-METH BA-CONV BCHTOL IN-LTRANGE IN-LPRANGE IN-UTRANGE IN-UPRANGE TA-LTRANGE TA-LPRANGE TA-UTRANGE TA-UPRANGE SIM-TOL P-SAVE-TOL BA-INI-TOL PS-FLASH

Input Language Description for PRES-RELIEF

pblockid ..... Pressure relief block ID

PROPERTIES Use to specify physical property calculations for the block.

OPSETNAME ..... Physical property option set to use in place of global default

HENRY-COMPS ..... Henry's constant component list ID

CHEMISTRY ..... ID of a CHEMISTRY paragraph

TRUE-COMPS ..... Electrolytes computation method:

TRUE-COMPS=YES	Uses true species simulation approach (Default)
TRUE-COMPS=NO	Uses apparent component in simulation approach

FREE-WATER ..... Free-water phase option set name. (See Chapter 8.)

SOLU-WATER ..... Method for calculating the K-value of water in the organic phase:

SOLU-WATER=0	Uses water solubility correlation. Vapor phase fugacity for water calculated by free-water phase option set.
SOLU-WATER=1	Uses water solubility correlation. Vapor phase fugacity for water calculated by primary option set.
SOLU-WATER=2	Uses water solubility correlation with a correction for unsaturated systems. Vapor phase fugacity for water calculated by primary option set.
SOLU-WATER=3	Uses primary option set. This method is not recommended for water-hydrocarbon systems unless water-hydrocarbon interaction parameters are available. (Default)

BLOCK-OPTIONS Use to override the diagnostic message levels and restart option, established by the DIAGNOSTICS and SIM-OPTIONS paragraphs. (See Chapter 45.)

PARAM Use to specify the calculation mode, scenario, vessel configuration, and optional convergence parameters. SCENARIO and DISCHARGE-PR are required.

SCENARIO ..... An event that, without pressure relief, would cause system pressure to rise above the maximum allowable working pressure:

SCENARIO=FIRE	Dynamic scenario with vessel exposed to external fire
SCENARIO=HEAT-INPUT	Dynamic scenario with fixed or variable heat flux into vessel
SCENARIO=FLOW-SPEC	Steady-state valve rating scenario with piping

	SCENARIO= VALVE-RATING	Steady-state simple valve rating scenario with no piping
CAPACITY	Determines whether the simulation is based on actual capacity of the hardware or on code capacity:	
	CAPACITY=CODE	Runs the simulation at code capacity (Default)
	CAPACITY=ACTUAL	Runs the simulation at actual capacity
NPHASE	Number of phases in the protected vessel:	
	NPHASE=1	One-phase calculation
	NPHASE=2	Vapor and liquid phases (Default)
	NPHASE=3	Vapor and two-liquid phases
DISENGAGEMENT	Model used to describe how vessel contents leave the vessel:	
	DISENGAGEMENT= HOMOGENEOUS	Homogeneous venting. The vapor fraction and composition leaving the vessel are the same as the vessel contents. (Default)
	DISENGAGEMENT= ALL-VAPOR	Vapor venting only. The composition of material leaving the vessel is the same as the composition of the vapor phase in the vessel.
	DISENGAGEMENT= ALL-LIQUID	Liquid venting only. The composition of material leaving the vessel is the same as the composition of the liquid phase in the vessel.
	DISENGAGEMENT= BUBBLY	DIERS bubbly/foamy venting
	DISENGAGEMENT= CHURN-TURBULENT	DIERS churn-turbulent venting
	DISENGAGEMENT= USER-SPEC	Homogeneous venting until vessel vapor fraction reaches specified value, then all-vapor venting
VFRAC	Homogeneous molar vapor fraction limit used when DISENGAGEMENT=USER-SPEC	
DISCHARGE-PR	Vent discharge pressure	
MAXIT	Maximum number of flash iterations (Default=30)	
TOL	Flash convergence tolerance (Default=$1x10^{-6}$)	
REACTION	Specifies whether or not reactions occur in the protected vessel. The vessel must be a horizontal, vertical, API, or spherical tank or a user-specified tank.	
	REACTION=NO	No reactions occur (Default)
	REACTION=YES	Reactions occur
VES-BASIS	Basis for the VESSEL-FRAC sentence:	
	VES-BASIS=MOLE	MOLE basis (Default)
	VES-BASIS=MASS	MASS basis
	VES-BASIS=STDVOL	Standard-liquid-volume basis
STRM-BASIS	Basis for the STREAM-FRAC sentence:	
	STRM-BASIS=MOLE	MOLE basis (Default)
	STRM-BASIS=MASS	MASS basis
	STRM-BASIS=STDVOL	Standard-liquid-volume basis
basis-FLOW	Flow rate for the FLOW-SPEC scenario, in MOLE, MASS, or STDVOL basis	
MAX-TIME	Upper limit on the simulation time for dynamic scenarios	

PRINT-TIME ..... Time interval between output points, printed in the block report. Aspen Plus uses this value when the vent is closed. It is also used when the vent is open, unless OPEN-TIME is specified.

ADD-POINTS ..... Specifies whether to generate extra output points at input profile points (DUTY-PROF sentence) and when the relief system opens or closes:

ADD-POINTS=YES	Generates extra points (Default)
ADD-POINTS=NO	Does not generate extra points

MAX-NPOINT ..... The number of output points generated if the upper limit on the simulation time is reached. Enter the next integer value greater than:

$$\frac{\text{MAX} - \text{TIME}}{\text{PRINT} - \text{TIME}} + 1$$

OPEN-TIME ..... Time interval between output points printed in the block report used when the relief system is open. Default uses PRINT-TIME value.

VENT-NPHASE ..... Number of phases in the relief system:

VENT-NPHASE=1	One-phase
VENT-NPHASE=2	Vapor and liquid phases (Default)
VENT-NPHASE=3	Vapor and two-liquid phases

VENT-PHASE ..... Phase in the relief system when VENT=NPHASE=1:

VENT-PHASE=V	Vapor (Default)
VENT-PHASE=L	Liquid

REFERENCE

Use to reference the stream whose composition will initialize the scenario. For FIRE and HEAT-INPUT scenarios, the initial vessel composition is taken from the referenced stream. For other scenarios, the composition of the inlet stream is taken from the referenced stream.

STREAM ..... Stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

VESSEL-FRAC

Use to specify the composition in the vessel for FIRE and HEAT-INPUT scenarios if the REFERENCE sentence is not used. You can specify the basis in MOLE, MASS, or STDVOL using VES-BASIS keyword in the PARAM sentence. Default is MOLE basis.

cid ..... Component ID

frac ..... Component fraction

STREAM-FRAC

Use to specify the composition of the inlet stream for the FLOW-SPEC and VALVE-RATING scenarios if the REFERENCE sentence is not used. You can specify the basis in MOLE, MASS, or STDVOL using STRM-BASIS keyword in the PARAM sentence. Default is MOLE basis.

cid ..... Component ID

frac ..... Component fraction

VESSEL

Use to specify vessel and vessel head geometry for dynamic simulations. MAWP and its corresponding temperature MAWP-TEMP are required for all vessel types.

VES-TYPE ..... Type of vessel:

VES-TYPE=HORIZONTAL	Horizontal cylindrical tank
VES-TYPE=VERTICAL	Vertical cylindrical tank
VES-TYPE=API-TANK	API tank
VES-TYPE=SPHERE	Spherical tank

	VES-TYPE=HX-SHELL	Heat-exchanger shell
	VES-TYPE= VESSEL-JACKET	Heating jacket around a vessel
	VES-TYPE=USER-SPEC	User-specified volume and area

MAWP ..... Maximum allowable working pressure. If you specified SCENARIO=FLOW-SPEC or VALVE-RATING, you cannot use MAWP.

MAWP-TEMP ..... Temperature at given MAWP. If you specified SCENARIO=FLOW-SPEC or VALVE-RATING, you cannot use MAWP-TEMP.

HEADS ..... Describes the heads on the ends of the vessel. Required when VES-TYPE=HORIZONTAL, VERTICAL, API-TANK, or HX-SHELL.

HEADS=FLANGED	Flanged and dished heads
HEADS=ELLIPSOIDAL	Ellipsoidal heads
HEADS=USER-SPEC	User-specified area and volume. You must also enter HEAD-AREA and HEAD-VOL.

HEAD-AREA..... Area of head. Allowed only when HEADS=USER-SPEC.

HEAD-VOL..... Volume of head. Allowed only when HEADS=USER-SPEC.

DIAMETER..... Vessel diameter. Required when VES-TYPE is not USER-SPEC.

LENGTH..... Vessel length. Required when VES-TYPE is not SPHERE or USER-SPEC.

MOUNT..... Describes how heat-exchanger is mounted. Required when VES-TYPE is HX-SHELL.

MOUNT=HORIZONTAL	Horizontal mount
MOUNT=VERTICAL	Vertical mount

JACKET-VOL..... Volume of vessel jacket. Required when VES-TYPE=VESSEL-JACKET.

VES-VOLUME..... Volume of user-specified vessel. Required when VES-TYPE=USER-SPEC.

VES-AREA ..... Area of vessel. Required when VES-TYPE=USER-SPEC.

VES-NECK-DIA ..... Vessel neck diameter

VES-NECK-DIR ..... Vessel neck direction:

VES-NECK-DIR= VERTICAL	Vertical neck (Default)
VES-NECK-DIR= HORIZONTAL	Horizontal neck

VES-NECK-LEN ..... Vessel neck length. A value of 0 indicates there is no vessel neck.

VES-NECK-CON ..... Vessel neck connection to the vessel:

VES-NECK-CON= ROUNDED	Rounded connection (Default)
VES-NECK-CON=SQUARE	Square connection
VES-NECK-CON= IN-PROJECTING	Inward projecting

VES-NECK-RUF..... Absolute roughness of the vessel neck (Default=1.5×10^{-4}ft, 0.04572 mm)

REDUCER-K..... Resistance coefficient for reducer between the vessel neck and the following length of pipe (Default=0.04)

EXPANDER-K..... Resistance coefficient for expander between the vessel neck and the following length of pipe (Default=0.04)

DEAD-VOL ..... Volume of vessel internal structures to be substracted from calculated vessel volume

CONDITIONS

Use to specify initial conditions for the dynamic scenarios or feed stream conditions for the steady state scenarios.

FILLAGE ..... Fraction of the volume of the tank which is liquid at the normal operating condition. Allowed for the FIRE and HEAT-INPUT scenarios.

PAD-COMP ..... Component to be used as pad-gas. If you use PAD-COMP, this material is added to the vessel to bring the pressure to the specified value. Allowed for FIRE and HEAT-INPUT scenarios.

VES-TEMP ..... Initial temperature in the vessel. Allowed for FIRE and HEAT-INPUT scenarios.

VES-PRES ..... Initial pressure in the vessel. Allowed for FIRE and HEAT-INPUT scenarios.

VES-VFRAC ..... Initial molar vapor fraction in the vessel. Allowed for FIRE and HEAT-INPUT scenarios.

VES-TFROM ..... Source of initial vessel temperature. Allowed for FIRE and HEAT-INPUT scenarios.

VES-TFROM= CALCULATE	Calculates initial temperature of vessel contents (Default)
VES-TFROM= FROM-STREAM	Takes initial temperature from referenced stream

VES-PFROM ..... Source of initial vessel pressure. Allowed for FIRE and HEAT-INPUT scenarios.

VES-PFROM= CALCULATE	Calculates initial pressure of vessel contents (Default)
VES-PFROM= FROM-STREAM	Takes initial pressure from referenced stream

VES-VFFROM ..... Source of initial vessel vapor fraction. Allowed for FIRE and HEAT-INPUT scenarios.

VES-VFFROM= CALCULATE	Calculates initial vapor fraction (Default)
VES-VFFROM= FROM-STREAM	Takes initial vapor fraction from referenced stream

STRM-TEMP ..... Temperature of the stream entering the relief system. Allowed for FLOW-SPEC and VALVE-RATING scenarios.

STRM-PRES ..... Pressure of the stream entering the relief system. Allowed for FLOW-SPEC and VALVE-RATING scenarios.

STRM-VFRAC ..... Vapor fraction of the stream entering the relief system. Allowed for the FLOW-SPEC and VALVE-RATING scenarios.

STRM-TFROM ..... Source of temperature of the stream entering the relief system. Allowed for FLOW-SPEC and VALVE-RATING scenarios.

STRM-TFROM= CALCULATE	Calculates temperature of the inlet stream (Default)
STRM-TFROM= FROM-STREAM	Takes temperature from the referenced stream

STRM-PFROM ..... Source of pressure of the stream entering the relief system. Allowed for FLOW-SPEC and VALVE-RATING scenarios.

STRM-PFROM= CALCULATE	Calculates pressure of the inlet stream (Default)

	STRM-PFROM=FROM-STREAM	Takes pressure from the referenced stream

STRM-VFFROM ..... Source of vapor fraction of the stream entering the relief system. Allowed for FLOW-SPEC and VALVE-RATING scenarios.

STRM-VFFROM=CALCULATE	Calculates vapor fraction of the inlet stream (Default)
STRM-VFFROM=FROM-STREAM	Takes vapor fraction from the referenced stream

REACTIONS

Use to specify the IDs of REACTIONS paragraphs to be included with the simulation of the vessel.

REACID ..... List of IDs of REACTIONS paragraphs. (See Chapter 6.)

FIRE

Use to enter parameters for the FIRE scenario.

STANDARD ..... Regulations from which to take FIRE scenario:

STANDARD=NFPA-30	Conform to NFPA 30 rules
STANDARD=API-520	Conform to API 520 rules
STANDARD=API-2000	Conform to API 2000 rules

ELEVATION ..... Height of the vessel above ground level (Default=0)

DRAINAGE ..... Allows the user to claim a credit for drainage. Allowed only when STANDARD=NFPA-30.

DRAINAGE=YES	Claims credit for drainage
DRAINAGE=NO	Does not claim credit for drainage (Default)

WATER-SPRAY ..... Allows the user to claim a credit for having a water spray. Allowed only when STANDARD=NFPA-30.

WATER-SPRAY=YES	Claims credit for water spray
WATER-SPRAY=NO	Does not claim credit for water spray (Default)

INSULATION ..... Allows the user to claim a credit for having an insulated vessel. You cannot use INSULATION if PORTABLE=YES.

INSULATION=YES	Claims credit for insulated vessel
INSULATION=NO	Does not claim insulation credit (Default)

PORTABLE..... Indicates whether the fire is under a portable tank. If so, different NFPA rules apply. Allowed only when STANDARD=NFPA-30.

PORTABLE=YES	Tank is portable
PORTABLE=NO	Tank is not portable (Default)

CREDIT-FACT ..... Allows the user to enter a credit factor instead of having PRES-RELIEF calculate it from other input. You cannot use CREDIT-FAC if you specified any individual credit factors using the keywords DRAINAGE, WATER-SPRAY, INSULATION, and INS-CREDIT. (Default=1)

EXTRA-AREA ..... Extra area for heat transfer. This value is added to the calculated vessel area.

FIRE-TIME ..... Duration of the fire around the vessel

INS-CREDIT ..... Insulation protection factor for API-520 and API-2000 or when INSULATION=YES

DR-AND-FF..... Credit factor for having drainage and fire-fighting equipment available. Allowed only when STANDARD=API-520.

DR-AND-FF=YES	Claims this credit factor
DR-AND-FF=NO	Does not claim this credit factor (Default)

LIQ-LEVEL Height of liquid in the vessel. Allowed only when VES-TYPE=HORIZONTAL, VERTICAL, API-TANK, or HX-SHELL and STANDARD=API-520.

DUTY-PROF Use to enter the time-varying duty profile for the HEAT-INPUT scenario. Linear interpolation is used for duties between the specified times.

time Time

duty Heat duty at the corresponding time

HEAT-INPUT Use to enter parameters for the HEAT-INPUT scenario. When you choose the HEAT-INPUT scenario, you can then specify DUTY or a time-varying duty profile (DUTY-PROF sentence) or TEMP, U, and AREA.

TEMP Temperature of material in the jacket

U Heat transfer coefficient

AREA Area for heat transfer

DUTY Heat duty

RELIEF-DEV Use to specify parameters for the relief devices.

DEVICE Type of relief device:

DEVICE=PSV	Safety relief valve (Default)
DEVICE=PSD	Rupture disk
DEVICE=ERV	Emergency relief vent
DEVICE=PIPE	Open vent pipe
DEVICE=PSV-PSD	Safety relief valve/rupture disk combination

PSV-SERVICE Service of safety relief valve. Required when DEVICE=PSV.

PSV-SERVICE="LIQUID"	Liquid service
PSV-SERVICE= "GAS/2-PHASE"	Gas or two-phase service

PSV-THROAT Safety relief valve throat diameter. Required when DEVICE=PSV.

PSV-IN-DIAM Safety relief valve inlet diameter. Required when DEVICE=PSV.

PSV-OUT-DIAM Safety relief valve outlet diameter. Required when DEVICE=PSV.

PSV-CD Safety relief valve discharge coefficient. Required when DEVICE=PSV.

PSV-OVER-PR Over-pressure factor for liquid service safety relief valve. Allowed only when PSV-SERVICE="LIQUID". (Default=1.1)

PSV-SETPOINT Differential setpoint for the safety relief valve. Defined as the pressure difference across the valve, which is needed for the valve to start opening. Required when DEVICE=PSV.

PSV-OPEN Parameter used to calculate the pressure at which the gas or two-phase service valve opens. The valve opens when the pressure across the valve reaches PSV-SETPOINT*PSV-OPEN.
Allowed only when PSV-SERVICE="GAS/2-PHASE". (Default=1.1)

PSV-CLOSE Parameter used to calculate the pressure at which the gas or two-phase service valve closes. The valve closes when the pressure across the valve reaches PSV-SETPOINT*PSV-CLOSE.
Allowed only when PSV-SERVICE="GAS/2-PHASE". (Default=0.93)

PSD-DIAM Rupture disk diameter. Required when DEVICE=PSD.

PSD-CD Discharge coefficient for rupture disk. Required when DEVICE=PSD and CAPACITY=CODE.

PSD-LD ..... Value of equivalent L/D used to model the rupture disk in the actual capacity run. Required when DEVICE=PSD, and CAPACITY=ACTUAL.

PSD-SETPOINT ..... Differential setpoint for the rupture disk. Defined as the pressure difference across the rupture disk, which is needed for the disk to break. Required when DEVICE=PSD.

ERV-DIAM ..... Diameter of emergency relief vent. Required when DEVICE=ERV.

ERV-SETPOINT..... Differential setpoint for the emergency relief vent. Defined as the pressure difference across the vent, which is needed for the vent to open. Required when DEVICE=ERV.

ERV-OVER-PR ..... Over-pressure factor. The vent completely opens when the pressure drop across it reaches ERV-OVER-PR*ERV-SETPOINT. (Default=1.1)

COMB-COEF..... Combination coefficient for PSV/PSD. If the combination is not certified a value of 0.9 is required by the ASME.

N-INLET-SECT..... Number of sections of pipe between the vessel neck and the relief device: 0, 1, or 2 (Default=0)

N-TAIL-SECT ..... Number of sections of pipe after the relief device: 0, 1, or 2 (Default=0)

INLET-PIPE Use to specify parameters for the inlet pipes. You must specify ACTUAL-DIAM, LENGTH, and CONNECTIONS. You can use up to two sections of pipe with the same or different diameters. You can also specify any fittings such as gate valves, elbows, and branched tees.

secno ..... Section number

ACTUAL-DIAM..... Actual pipe diameter

LENGTH..... Length of pipe

CONNECTIONS..... Type of connection between pipe lengths:

CONNECTIONS= FLANGED-WELDED	Flanged or welded connection (Default)
CONNECTIONS= SCREWED	Screwed connection

ELEVATION ..... Net vertical change in distance between the inlet and outlet of the piping section

ELBOWS..... Number of 90° elbows in the pipe

STRAIGHT-TEE..... Number of straight tees in the pipe

BRANCHED-TEE..... Number of branched tees in the pipe

GATE-VALVES ..... Number of gate valves in the pipe

BUTTERFLY-VA..... Number of butterfly valves in the pipe

VALVE-AREA ..... Valve flow area

VALVE-COEFF..... Valve flow coefficient

CONTROL-CV..... Valve constant for control valve in the pipe. Enter 0 if none.

MISC-L-D ..... Miscellaneous L/D for other elements in the pipe

TAMBIN ..... Ambient temperature at the pipe inlet

TAMBOUT..... Ambient temperature at the pipe outlet

U ..... Overall heat transfer coefficient

REDUCER-K ..... Resistance coefficient for reducer between this pipe and the following length of pipe (Default=0.04)

EXPANDER-K ..... Resistance coefficient for expander between this pipe and the following length of pipe (Default=0.04)

ROUGHNESS ..... Pipe absolute roughness (Default=$1.5x10^{-4}$ ft, .04572 mm)

TAIL-PIPE

Use to specify parameters for the tail pipe section(s) following the relief device. You must specify ACTUAL-DIAM, LENGTH, and CONNECTIONS. You can use up to two sections of pipe with the same or different diameters. You can also specify any fittings such as gate valves, elbows, and branched tees.

secno ..... Section number

ACTUAL-DIAM ..... Actual pipe diameter

LENGTH ..... Length of pipe

CONNECTIONS ..... Type of connection between pipe lengths:

CONNECTIONS= FLANGED-WELDED	Flanged or welded connection (Default)
CONNECTIONS= SCREWED	Screwed connection

ELEVATION ..... Net vertical change in distance between the inlet and outlet of the piping section

ELBOWS ..... Number of 90° elbows in the pipe

STRAIGHT-TEE ..... Number of straight tees in the pipe

BRANCHED-TEE ..... Number of branched tees in the pipe

GATE-VALVES ..... Number of gate valves in the pipe

BUTTERFLY-VA ..... Number of butterfly valves in the pipe

VALVE-AREA ..... Valve flow area

VALVE-COEFF ..... Valve flow coefficient

CONTROL-CV ..... Valve constant for control valve in the pipe. Enter 0 if none.

MISC-L-D ..... Miscellaneous L/D for other elements in the pipe

TAMBIN ..... Ambient temperature at the pipe inlet

TAMBOUT ..... Ambient temperature at the pipe outlet

U ..... Overall heat transfer coefficient

REDUCER-K ..... Resistance coefficient for reducer between this pipe and the following length of pipe (Default=0.04)

EXPANDER-K ..... Resistance coefficient for expander between this pipe and the following length of pipe (Default=0.04)

ROUGHNESS ..... Pipe absolute roughness (Default=$1.5x10^{-4}$ ft, 0.04572 mm)

STOP

Use to specify stop criteria. Enter one STOP sentence for each stop criterion. If you specify more than one stop criterion, the simulation is halted when any one of the stop criteria is reached. You can specify the stopping criterion variable to reach its specified value FROM-ABOVE or FROM-BELOW.

stopno ..... Stop criterion number

location ..... Location for the variable:

	VESSEL	In vessel
	ACCUMULATOR	In vent accumulator
	VENT	In continuous vent
variable	Stop criterion variable:	
	TIME	Reaction time
	MASS-FRAC	Mass fraction of a component specified by COMP
	MOLE-FRAC	Mole fraction of a component specified by COMP
	CONVERSION	Conversion of a component specified by COMP
	MOLES	Total moles inside the reactor or vent accumulator
	MASS	Total mass inside the reactor or vent accumulator
	TEMP	Reactor temperature
	MOLE-FLOW	Vent mole flow rate
	MASS-FLOW	Vent mass flow rate
	VFRAC	Vapor fraction in the vessel
	PRES	Pressure in the vessel
value	Value of variable at which to stop simulation	
from	**FROM-ABOVE**	Terminates simulation when variable value is reached from above
	FROM-BELOW	Terminates simulation when variable value is reached from below
COMP	Component ID. Required when variable is MOLE-FRAC, MASS-FRAC, or CONVERSION.	
SUBSTREAM	Substream ID. Required when variable is MOLE-FRAC or CONVERSION.	

RULES

Use to specify design rules, such as limitations on inlet and tail pipe pressure losses and maximum vessel pressure.

IN-MAXFAC	Maximum allowed inlet piping pressure loss as a percentage of differential set pressure. Calculated at 10% over-pressure or maximum pressure if 10% over-pressure is not reached. (Default=3%)	
TAIL-ALLFAC	Maximum allowed tail pipe pressure drop as a percentage of differential set pressure. Calculated at 10% over-pressure or maximum pressure if 10% over-pressure is not reached.	
RESPOND	The 97% rule. If the 97% rule is used the pressure drop across the valve must be greater than or equal to 97% of the valve's differential set pressure.	
	RESPOND=YES	Applies 97% rule
	RESPOND=NO	Does not apply 97% rule
EQP-MAXFAC	Maximum allowed vessel pressure as a percentage of MAWP	
EQP-MAXPRE	Maximum allowed vessel pressure	
SPCHANGE	Differential set pressure option:	
	SPCHANGE=YES	Differential set pressure changes as back pressure changes
	SPCHANGE=NO	Differential set pressure does not change as back pressure changes (Default)

REPORT

Use to override the default report options. (See Chapter 11.)

reportopt Report options:

	NOREPORT	Suppresses the the block report
	NEWPAGE	Specifies that each block report is to begin on a new page
	NOINPUT	Suppresses the summary of user input and system defaults
	NORESULTS	Suppresses the block results

CONVERGENCE Use to enter simulation methods, flash table parameters, and optional convergence parameters, and pipe friction and holdup methods.

SFLASH-MAXIT	Maximum number of iterations for constant entropy flash (Default=30)	
SFLASH-TOL.....	Tolerance for constant entropy flash (Default=$1x10^{-10}$)	
BUBBLY-C0	Coefficient for DIERS bubbly disengagement option (Default=1.01)	
CHURN-C0.....	Coefficient for DIERS churn-turbulent disengagement option (Default=1)	
VALVE-SFLASH.....	**VALVE-SFLASH=YES**	Performs constant entropy flash calculations in the valve
	VALVE-SFLASH=NO	Does not perform constant enthalpy flash calculations in the valve (Default)
CVT-SFLASH.....	**CVT-SFLASH=YES**	Performs constant entropy flash calculations when converting between flowing and stagnation pressure
	CVT-SFLASH=NO	Does not perform constant enthalpy flashes (Default)
VAL-SIMPSON.....	Method for modeling the valve:	
	VAL-SIMPSON=YES	Uses Simpson's shortcut method when modeling the valve (Default)
	VAL-SIMPSON=NO	Performs rigorous flash calculations when modeling the valve
CVT-SIMPSON.....	**CVT-SIMPSON=YES**	Uses Simpson's shortcut method when converting between flowing and stagnation pressure (Default)
	CVT-SIMPSON=NO	Performs rigorous flash calculations when converting between flowing and stagnation pressure
INLET-TABLE	Flash tables option for speeding up vessel neck and inlet pipe calculations	
	INLET-TABLE=YES	Uses flash tables (Default)
	INLET-TABLE =NO	Does not use flash tables
INLET-NT	Number of temperature points for the vessel neck and inlet pipe flash tables (Default=5)	
INLET-NP.....	Number of pressure points for the vessel neck and inlet pipe flash tables (Default=5)	
TAIL-TABLE.....	Flash tables option for speeding up tail pipe calculations:	
	TAIL-TABLE=YES	Uses flash tables (Default)
	TAIL-TABLE=NO	Does not use flash tables
TAIL-NT	Number of temperature points for the tail pipe flash tables (Default=5)	
TAIL-NP.....	Number of pressure points for the tail pipe flash tables (Default=5)	
DEVICE-ONLY	Pipe modeling option:	

	DEVICE-ONLY=YES	Does not model vessel neck, inlet and tail pipes during dynamic simulation
	DEVICE-ONLY=NO	Models piping during dynamic simulations (Default)
PRES-TOL.....	Convergence tolerance in pressure convergence loop (Default=$1x10^{-4}$)	
FLOW-TOL.....	Convergence tolerance in flow convergence loop (Default=$1x10^{-4}$)	
FRIC-DOWNHILL.....	Two-phase frictional pressure-drop correlation option for downhill flow. Use when inclination angles are less than -2 degrees from horizontal.	
	FRIC-DOWNHILL= BEGGS-BRILL	Beggs and Brill (Default)
	FRIC-DOWNHILL=DARCY	Darcy. Assumes no slip.
	FRIC-DOWNHILL=SLACK	Slack
FRIC-HORIZ.....	Two-phase frictional pressure-drop correlation option for horizontal flow. Use when the inclination angles range between -2 and +2 degrees from horizontal.	
	FRIC-HORIZ= BEGGS-BRILL	Beggs and Brill (Default)
	FRIC-HORIZ=DARCY	Darcy. Assumes no slip.
	FRIC-HORIZ=DUKLER	Dukler
	FRIZ-HORIZ=LOCK-MART	Lockhart-Martinelli
FRIC-INCL.....	Two-phase frictional pressure-drop correlation option for inclined flow. Use when inclination angles range between +2 and +45 degrees from horizontal.	
	FRIC-INCL=AWR	Angel-Welchon-Ros
	FRIC-INCL=BEGGS-BRILL	Beggs and Brill (Default)
	FRIC-INCL=DARCY	Darcy. Assumes no slip.
	FRIC-INCL=DUKLER	Dukler
	FRIC-INCL=H-BROWN	Hagedorn-Brown
	FRIC-INCL=ORKI	Orkiszewski
FRIC-VERTICA	Two-phase frictional pressure-drop correlation option for vertical flow. Use when inclination angles are greater than +45 degrees from horizontal.	
	FRIC-VERTICA-AWR	Angel-Welchon-Ros
	FRIC-VERTICA= BEGGS-BRILL	Beggs and Brill (Default)
	FRIC-VERTICA=DARCY	Darcy. Assumes no slip.
	FRIC-VERTICA=H-BROWN	Hagedorn-Brown
	FRIC-VERTICA=ORKI	Orkiszewski
HOLDUP-DOWNH	Two-phase liquid holdup correlation option for downhill flow. Use when inclination angles are less than -2 degrees from horizontal.	
	HOLDUP-DOWNH=BEGGS -BRILL	Beggs and Brill (Default)
	HOLDUP-DOWNH=SLACK	Slack
HOLDUP-HORIZ	Two-phase liquid holdup correlation option for horizontal flow. Use when inclination angles range between -2 and +2 degrees from horizontal.	
	HOLDUP-HORIZ= BEGGS-BRILL	Beggs and Brill (Default)

	HOLDUP-HORIZ=EATON	Eaton
	HOLDUP-HORIZ=HOOG	Hoogendorn
	HOLDUP-HORIZ=HUGH	Hughmark
	HOLDUP-HORIZ= LOCK-MART	Lockhart-Martinelli
HOLDUP-INCL	Two-phase liquid holdup correlation option for inclined flow. Use when inclination angles range between +2 and +45 degrees from horizontal.	
	HOLDUP-INCL=AWR	Angel-Welchon-Ros
	HOLDUP-INCL= BEGGS-BRILL	Beggs and Brill (Default)
	HOLDUP-INCL=FLANIGAN	Flanigan
	HOLDUP-INCL=H-BROWN	Hagedorn-Brown
	HOLDUP-INCL=ORKI	Orkiszewski
HOLDUP-VERTI	Two-phase liquid holdup correlation option for vertical flow. Use when inclination angles are greater than +45 degrees from horizontal.	
	HOLDUP-VERT=AWR	Angel-Welchon-Ros
	HOLDUP-VERT= BEGGS-BRILL	Beggs and Brill (Default)
	HOLDUP-VERT= H-BROWN	Hagedorn-Brown
	HOLDUP-VERT=ORKI	Orkiszewski
STOP-CYCLING	Option to stop cycling of relief device:	
	STOP-CYCLING=YES	Stops the simulation when excessive opening and closing of the relief device occurs (Default)
	STOP-CYCLING=NO	Does not stop the simulation
MAX-NCYCLE	Number of openings and closings of the relief device within CYCLE-TIME after which simulation will be terminated. (Default=3)	
CYCLE-TIME	Amount of time within which MAX-NCYCLE must occur for the simulation to be terminated (Default=2 sec)	
ATMOS-PRES	Local absolute atmospheric pressure (Default=14.69595 psia)	
BA-H0	Initial step-size (in seconds) used by the vessel integration routine (Default=0.1)	
BA-HMXUSR	Maximum step-size (in seconds) allowed in the vessel integration routine	
BA-RINTOL	Convergence tolerance used by the vessel integration routine (Default=$1x10^{-4}$)	
BA-CORR-METH	Corrector convergence method used by vessel integration routine:	
	BA-CORR-METH=DIRECT	Uses direct substitution
	BA-CORR-METH= NEWTON	Uses Newton method (Default)
VA-H0	Initial step-size used by the valve integration routine as a fraction of the maximum possible pressure change (Default=0.01)	
VA-HMXUSR	Maximum relative step-size allowed in the valve integration routine	
VA-RINTOL	Convergence tolerance used by the valve integration routine (Default=$1x10^{-4}$)	
VA-CORR-METH	Corrector convergence method used by valve integration routine:	

	VA-CORR-METH=DIRECT	Uses direct substitution method
	VA-CORR-METH= NEWTON	Uses Newton method (Default)

CV-H0 ..... Initial relative step-size used by the valve integration routine, which converts flowing between stagnation pressure (Default=0.01)

CV-HMXUSR ..... Maximum step-size allowed in the integration routine, which converts flowing between stagnation pressure

CV-RINTOL..... Convergence tolerance used by the integration routine, which converts between flowing and stagnation pressure (Default=$1x10^{-4}$)

CV-CORR-METH..... Corrector convergence method used by integration routine, which converts between flowing and stagnation pressure:

CV-CORR-METH=DIRECT	Uses direct substitution
CV-CORR-METH= NEWTON	Uses Newton method (Default)

IN-H0..... Initial step-size used by the inlet pipe and vessel neck integration routines. Enter as a fraction of the total length. (Default=0.1)

IN-HMXUSR ..... Maximum step-size allowed in the inlet pipe and vessel neck integration routines

IN-RINTOL..... Convergence tolerance used by the vessel neck and inlet pipe integration routines (Default=$1x10^{-4}$)

IN-CORR-METH ..... Corrector convergence method used by vessel neck and inlet pipe integration routines:

IN-CORR-METH=DIRECT	Uses direct substitution method
IN-CORR-METH=NEWTON	Uses Newton method (Default)

TA-H0 ..... Initial step-size used by the tail pipe integration routine. Enter as a fraction of the total length. (Default=0.1)

TA-HMXUSR ..... Maximum step-size allowed in the tail pipe integration routine

TA-RINTOL..... Convergence tolerance used by the tail pipe integration routine (Default=$1x10^{-4}$)

TA-CORR-METH..... Corrector convergence method used by tail pipe integration routine:

TA-CORR-METH=DIRECT	Uses direct substitution method
TA-CORR-METH= NEWTON	Uses Newton method (Default)

BA-CONV..... Solution scheme used in batch pressure convergence:

BA-CONV=ARCONS	Numerical search using standard secant method (Default)
BA-CONV=ROOT1N	Numerical search using modified secant method
BA-CONV=NEWTON	Numerical search using Newton method

BCHTOL..... Convergence tolerance for the bubbly or churn-turbulent vapor fraction calculation loop (Default=0.001)

IN-LTRANGE ..... Factor used in calculating the lowest temperature for the inlet- pipe flash table. The lowest temperature is (1-*IN-LTRANGE*)*(rigorous lowest temperature). (Default=0.1)

IN-LPRANGE ..... Factor used in calculating the lowest pressure for the inlet-pipe flash table. The lowest pressure is (1-*IN-LPRANGE*)*(rigorous lowest pressure). (Default=0.1)

IN-UTRANGE ..... Factor used in calculating the highest temperature for the inlet-pipe flash table. The highest temperature is (1+*IN-UTRANGE*)*(rigorous highest temperature). (Default=0.1)

IN-UPRANGE ..... Factor used in calculating the highest temperature for the inlet-pipe flash table. The highest temperature is (1+*IN-UPRANGE*)*(rigorous highest pressure). (Default=0.1)

TA-LTRANGE ..... Factor used in calculating the lowest temperature for the tail- pipe flash table. The lowest temperature is (1-*TA-LTRANGE*)*(rigorous highest temperature). (Default=0.1)

TA-LPRANGE ..... Factor used in calculating the lowest pressure for the tail-pipe flash table. The lowest pressure is (1-*TA-LPRANGE*)*(rigorous lowest pressure). (Default=0.1)

TA-UTRANGE ..... Factor used in calculating the highest temperature for the tail- pipe flash table. The highest temperature is (1+*TA-UTRANGE*)*(rigorous highest temperature). (Default=0.1)

TA-UPRANGE ..... Factor used in calculating the highest pressure for the tail-pipe flash table. The highest pressure is (1+*TA-UPRANGE*)*(rigorous highest pressure). (Default=0.1)

SIM-TOL ..... Simpson parameter recalculation factor. SIM-TOL is used repeatedly until the inlet temperature varies by more than the specified tolerance. (Default=0.001)

P-SAVE-TOL ..... Vessel pressure tolerance used to determine when to calculate a new vent flow rate during dynamic simulation (Default=0.01)

BA-INI-TOL ..... Convergence tolerance for initial vessel conditions used in dynamic scenarios (Default=0.001)

PS-FLASH ..... For constant entropy flash calculations, determines which algorithm to use:

PS-FLASH=DIRECT	Use direct call to Flash (Default)
PS-FLASH=INDIRECT	Perform a series of PQ flashes until the specified entropy is obtained

Accessing Variables in PRES-RELIEF

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for a PRES-RELIEF block.

Block Input

Sentence	Variables	ID1
PARAM	VFRAC, DISCHARGE-PR, MAXIT, TOL, MAX-TIME, PRINT-TIME, OPEN-TIME	—
VESSEL	MAWP, VES-NECK-DIA, VES-NECK-LEN REDUCER-K, EXPANDER-K, DEAD-VOL, DIAMETER, LENGTH, JACKET-VOL, VES-VOLUME, VES-AREA, HEAD-AREA, HEAD-VOL	—
CONDITIONS	STRM-TEMP, VES-TEMP, VES-PRES, VES-VFRAC, FILLAGE, STRM-PRES, STRM-VFRAC	—
FIRE	ELEVATION, EXTRA-AREA, FIRE-TIME, INS-CREDIT, CREDIT-FACT	—
HEAT-INPUT	TEMP, AREA, U, DUTY	—
RELIEF-DEV	PSV-SETPOINT, PSV-THROAT, PSV-IN-DIAM, PSV-OUT-DIAM, PSV-CD, PSV-OVER-PR, PSV-OPEN, PSV-CLOSE, COMB-COEF, ERV-DIAM, ERV-OVER-PR, ERV-SETPOINT, PSD-DIAM, PSD-CD, PSD-SETPOINT, PSD-LD	—
INLET-PIPE	ACTUAL-DIAM, LENGTH, ELEVATION, ELBOWS, STRAIGHT-TEE, BRANCHED-TEE, GATE-VALVES, BUTTERFLY-VA, VALVE-AREA, TAMBIN, TAMBOUT, U, CONTROL-CV, MISC-L-D, REDUCER-K, EXPANDER-K	indexno
TAIL-PIPE	ACTUAL-DIAM, LENGTH, ELEVATION, ELBOWS, STRAIGHT-TEE, BRANCHED-TEE, GATE-VALVES, BUTTERFLY-VA, VALVE-AREA, TAMBIN, TAMBOUT, U, CONTROL-CV, MISC-L-D, REDUCER-K, EXPANDER-K	indexno
STOP	VALUE	indexno
RULES	IN-MAXFAC, TAIL-ALLFAC, EQP-MAXFAC, EQP-MAXPRE	—
CONVERGENCE	SFLASH-TOL, BUBBLY-CO, CHURN-CO, INLET-NT, INLET-NP, TAIL-NT, TAIL-NP, PRES-TOL, FLOW-TOL, MAX-NCYCLE, CYCLE-TIME, ATMOS-PRES	—

Block Results

Description	Sentence	Variable	ID1
Calculated vessel volume	RESULTS	CALC-VOLUME	—
Calculated vessel wet area	RESULTS	CALC-AREA	—
Total simulation time	RESULTS	TOTAL-TIME	—
Initial vessel vapor fraction	RESULTS	VF-INIT	—
Maximum vessel temperature	RESULTS	MAX-TEMP	—
Initial vessel pressure	RESULTS	INIT-PRES	—
Initial vessel temperature	RESULTS	INIT-TEMP	—
Maximum vessel pressure	RESULTS	MAX-PRES	—
Maximum molar flow rate through pressure relief system	RESULTS	MAX-FLOW	—
Pressure drop through vessel neck and inlet piping at 10% over-pressure	RESULTS	INLET-DELTAP	—
Allowed pressure drop through vessel neck and inlet piping at 10% over-pressure	RESULTS	INCOD-DELTAP	—
Pressure drop through tail pipe at 10% over-pressure	RESULTS	TAIL-DELTAP	—
Allowed pressure drop through tail pipe at 10% over-pressure	RESULTS	TACOD-DELTAP	—
Calculated mass flow rate through pressure relief system	RESULTS	MASS-OUT	—
Calculated molar flow rate through pressure relief system	RESULTS	MOLE-OUT	—
Calculated volumetric flow rate through pressure relief system	RESULTS	VOL-OUT	—
Calculated heat input for fire scenario	RESULTS	Q-FIRE	—
Calculated credit factor for fire scenario	RESULTS	FIRE-FACTOR	—
Calculated pressure along the venting system	PROFILE	SS-PRES	locno
Calculated temperature along the venting system	PROFILE	SS-TEMP	locno
Calculated vapor fraction along the venting system	PROFILE	SS-VFRAC	locno
Calculated enthalpy along the venting system	PROFILE	SS-ENTH	locno
Calculated density along the venting system	PROFILE	SS-DENSITY	locno
Calculated vessel enthalpy	GENPROF	VES-ENTHALPY	timeno
Calculated vessel pressure	GENPROF	VES-PRESS	timeno
Calculated vessel temperature	GENPROF	VES-TEMP	timeno
Calculated vessel vapor fraction	GENPROF	VES-VFRAC	timeno
Calculated time	GENPROF	VES-TIME	timeno
Calculated vent accumulator enthalpy	GENPROF	ACC-ENTHALPY	timeno
Calculated vent molar flow rate	GENPROF	VENT-FLOW	timeno
Calculated vessel total mass	GENPROF	VES-MASS	timeno
Calculated vent accumulator total mass	GENPROF	ACC-MASS	timeno

40 Physical Property Tables

This chapter describes the input language for specifying physical property tables.

Use the PROP-TABLE paragraph to generate:

- Property tables.
- Flashcurve tables.
- PT Envelope tables.
- Residue curves.

Property Tables

Input Language for PROPS

```
PROP-TABLE    tableid    PROPS
DESCRIPTION   "a property table description – up to 64 characters in quotes"
PROPERTIES    opsetname    keyword=value
```

Optional keywords:

FREE-WATER SOLU-WATER HENRY-COMPS CHEMISTRY TRUE-COMPS

```
BLOCK-OPTIONS    keyword=value
```

Optional keywords:

SIM-LEVEL PROP-LEVEL FREE-WATER

```
STREAM    sid
basis-FLOW    cid    flow  /  ...
STATE    keyword=value
```

Optional keywords:

TEMP PRES

```
VARY    varname    keyword=value
```

Varnames:

TEMP PRES basis-FRAC basis-FLOW

Keywords:

COMP SUBSTREAM

```
RANGE    { LIST = value – list }
         { keyword = value     }
```

Keywords:

LOWER UPPER { **NPOINT** / **INCR** }

```
TABULATE    "heading"    PROPERTIES=propsetid-list    keyword=value
```

Optional keywords:

PRINT-PLOT HIGH-PRECISION LINES X-SCALE Y-SCALE
WIDE GRID INTERPOLATE

Input Language Description for PROPS

tableid ..... Property table ID

DESCRIPTION

A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the PROP-TABLE paragraph report.

PROPERTIES Use to replace the flowsheet property specifications. Any option set entered here must also be named in the PROPERTIES paragraph. (See Chapter 8.)

BLOCK-OPTIONS Use to override the diagnostic message levels established by the DIAGNOSTICS paragraph. (See Chapter 45.) For mixtures defined by the basis-FLOW sentence, you can use BLOCK-OPTIONS to override the free-water option established by the SIM-OPTIONS paragraph. (See Chapter 45.)

STREAM Use to reference a stream from a simulation. Do not use the STREAM sentence if you used the basis-FLOW sentence.

sid	Stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

basis-FLOW Use to establish sets of pure components, or to define mixtures on a MOLE, MASS, or STDVOL basis. When using basis-FLOW to establish a set of pure components, component flows are not used, but you must still enter a value greater than zero in the flows position. You cannot use the basis-FLOW sentence if you used the STREAM sentence.

cid	Component ID
flow	Flow rate on a MOLE, MASS, or STDVOL basis

STATE Use to specify state variable values when one or both of the two required variables, temperature or pressure, are not identified as independent variables in a VARY sentence. You cannot use the STATE sentence if you use the STREAM sentence.

TEMP	Temperature
PRES	Pressure

VARY Use to specify an independent variable that is varied over a range. You must enter at least one VARY sentence. You can use up to five VARY sentences. However, when print-plots are generated, you can use only one VARY sentence. If basis-FRAC is varied in a VARY sentence, basis-FLOW or a basis-FRAC of a different basis cannot also be varied in the same table. STDVOL basis is not allowed for CISOLID substream. For NC substream, MASS basis is the only allowed basis. You must enter a RANGE sentence with each VARY sentence.

varname	**TEMP**	Temperature
	PRES	Pressure
	basis-FRAC	Component fraction on a MOLE, MASS, or STDVOL basis
	basis-FLOW	Component flow on a MOLE, MASS, or STDVOL basis

COMP	Component ID. Required for basis-FRAC and basis-FLOW.
SUBSTREAM	Substream ID. Use for basis-FRAC and basis-FLOW. (Default=MIXED)

RANGE Use to specify independent variable values, either as a list of values, or over a range with a given number of increments or a given increment size. You must enter a RANGE sentence with each VARY sentence. For basis-FRAC and basis-FLOW, the values assigned by RANGE override the values in a basis-FLOW sentence or a referenced stream. When a range is applied to basis-FRAC for one or more components, the fractions of all other components are normalized by a common factor. In a RANGE sentence you can use only one of the following keywords: LIST, NPOINT, and INCR.

LIST	List of independent variable values
LOWER	Lower limit of a range
UPPER	Upper limit of a range
NPOINT	Number of points including LOWER and UPPER

INCR	Increment size between points	

TABULATE

Use to specify the properties to be tabulated. You must enter the TABULATE sentence. You must specify all desired properties, even state variables (for example, temperature) and composition (for example, mole fraction), or they will not be tabulated. The TABULATE sentence can also be used to generate print-plots and to specify plot options.

heading.....	String of up to 60 characters enclosed in quotes	
PROPERTIES	List of property set IDs for the properties to be tabulated. (See Chapter 41.)	
PRINT-PLOT.....	**PRINT-PLOT=YES**	Generates print-plots
	PRINT-PLOT=NO	Does not generate print-plots (Default)
HIGH-PRECISION	**HIGH-PRECISION=YES**	Prints seven significant digits in tables
	HIGH-PRECISION=NO	Prints five significant digits in tables (Default)
LINES.....	Number of rows of values to print in tables before printing a grid line. If LINES=0, no grid lines are printed. Must be between 0 and 35. (Default=5)	
X-SCALE.....	**X-SCALE=STANDARD**	Uses linear scale on horizontal axis of plots (Default)
	X-SCALE=INVERSE	Uses inverse scale on horizontal axis of plots
Y-SCALE.....	**Y-SCALE=STANDARD**	Uses linear scale on vertical axis of plots (Default)
	Y-SCALE=INVERSE	Uses inverse scale on vertical axis of plots
	Y-SCALE=LOG	Uses logarithmic scale on vertical axis of plots
WIDE, GRID, INTERPOLATE	Plot options. Use to override defaults established by the PLOT-OPTIONS paragraph. (See Chapter 46.)	

Flashcurve Tables

Input Language for FLASHCURVE

```
PROP-TABLE    tableid    FLASHCURVE
DESCRIPTION    "a property table description – up to 64 characters in quotes"
PROPERTIES    opsetname    keyword=value
```

Optional keywords:

FREE-WATER SOLU-WATER HENRY-COMPS CHEMISTRY TRUE-COMPS

```
BLOCK-OPTIONS    keyword=value
```

Optional keywords:

SIM-LEVEL PROP-LEVEL FREE-WATER

```
STREAM    sid    FLASH-CODE=value
basis-FLOW    cid    flow  /  . . .
STATE    keyword=value
```

Optional keywords:

TEMP PRES VFRAC

VARY	**varname**	*keyword=value*

Varnames:

TEMP PRES VFRAC DUTY basis-FRAC basis-FLOW

Keywords:

COMP SUBSTREAM

RANGE	$\left\{\begin{matrix}\textbf{LIST} = \textbf{value} - \textbf{list} \\ \textit{keyword} = \textit{value}\end{matrix}\right\}$

Keywords:

LOWER UPPER $\left\{\begin{matrix}\textbf{NPOINT} \\ \textbf{INCR}\end{matrix}\right\}$

PARAM	*keyword = value*

Optional keywords:

NPHASE MAXIT TOL

TABULATE	**"heading"**	**PROPERTIES=propsetid-list**	*keyword=value*

Optional keywords:

PRINT-PLOT HIGH-PRECISION LINES X-SCALE Y-SCALE WIDE GRID INTERPOLATE

Input Language Description for FLASHCURVE

tableid ..... Property table ID

DESCRIPTION A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the PROP-TABLE paragraph report.

PROPERTIES Use to replace the flowsheet property specifications. Any option set entered here must also be named in the PROPERTIES paragraph. (See Chapter 8.)

BLOCK-OPTIONS Use to override the diagnostic message levels established by the DIAGNOSTICS paragraph. (See Chapter 45.) For mixtures defined by the basis-FLOW sentence, you can use BLOCK-OPTIONS to override the free-water option established by the SIM-OPTIONS paragraph. (See Chapter 45.)

STREAM Use to reference a stream from a simulation. Do not use the STREAM sentence if you used the basis-FLOW sentence.

sid..... Stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

FLASH-CODE ..... Use to specify what type of flash to perform when one or both of the two required state variables (TEMP, PRES, VFRAC, and DUTY) are not identified as independent variables in the VARY sentence.

FLASH-CODE=PH	PH flash
FLASH-CODE=TP	TP flash
FLASH-CODE=PV	PV flash
FLASH-CODE=TH	TH flash
FLASH-CODE=TV	TV flash

basis-FLOW Use to establish sets of pure components, or to define mixtures on a MOLE, MASS, or STDVOL basis. When using basis-FLOW to establish a set of pure components, component flows are not used, but you must still enter a value greater than zero in the flows position. You cannot use the basis-FLOW sentence if you used the STREAM sentence.

cid..... Component ID

flow ..... Flow rate on a MOLE, MASS, or STDVOL basis

STATE Use to specify state variable values when one or both of the two required variables are not identified as independent variables in a VARY sentence. You cannot use the STATE sentence if you used the STREAM sentence.

TEMP..... Temperature

PRES..... Pressure

VFRAC..... Molar vapor fraction

VARY Use to specify an independent variable that is varied over a range. You must enter at least one VARY sentence. You can use up to five VARY sentences. However, when print-plots are generated, you can use only one VARY sentence. If basis-FRAC is varied in a VARY sentence, basis-FLOW or a basis-FRAC of a different basis cannot also be varied in the same table. STDVOL basis is not allowed for CISOLID substream. For NC substream, MASS basis is the only allowed basis. You must enter a RANGE sentence with each VARY sentence.

varname	**TEMP**	Temperature
	PRES	Pressure
	VFRAC	Molar vapor fraction
	DUTY	Heat duty
	basis-FRAC	Component fraction on a MOLE, MASS, or STDVOL basis
	basis-FLOW	Component flow on a MOLE, MASS, or STDVOL basis

COMP ..... Component ID. Required for basis-FRAC and basis-FLOW.

SUBSTREAM ..... Substream ID. Use for basis-FRAC and basis-FLOW. (Default=MIXED)

RANGE Use to specify independent variable values, either as a list of values, or over a range with a given number of increments or a given increment size. You must enter a RANGE sentence with each VARY sentence. For basis-FRAC and basis-FLOW, the values assigned by RANGE override the values in a basis-FLOW sentence or a referenced stream. When a range is applied to basis-FRAC for one or more components, the fractions of all other components are normalized by a common factor. In a RANGE sentence, you can use only one of the following keywords: LIST, NPOINT, and INCR.

LIST..... List of independent variable values

LOWER..... Lower limit of a range

UPPER..... Upper limit of a range

NPOINT..... Number of points including LOWER and UPPER

INCR..... Increment size between points

PARAM Use to specify NPHASE when a basis-FLOW sentence is used.

NPHASE	**NPHASE=2**	Two-phase flash (Default)
	NPHASE=3	Three-phase flash

MAXIT..... Maximum number of iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

TOL	Convergence tolerance. (Default=value established by SIM-OPTIONS paragraph.) (See Chapter 45.)	

TABULATE

Use to specify the properties to be tabulated. You must enter the TABULATE sentence. You must specify all desired properties, even state variables (such as temperature) and composition (such as mole fraction), or they will not be tabulated. You can also use the TABULATE sentence to generate print-plots and to specify plot options.

heading	String of up to 60 characters enclosed in quotes	
PROPERTIES	List of property set IDs for the properties to be tabulated. (See Chapter 41.)	
PRINT-PLOT	**PRINT-PLOT=YES**	Generates print-plots
	PRINT-PLOT=NO	Does not generate print-plots (Default)
HIGH-PRECISION	**HIGH-PRECISION=YES**	Prints seven significant digits in tables
	HIGH-PRECISION=NO	Prints five significant digits in tables (Default)
LINES	Number of rows of values to print in tables before printing a grid line. If LINES=0, no grid lines are printed. Must be between 0 and 35. (Default=5)	
X-SCALE	**X-SCALE=STANDARD**	Uses linear scale on horizontal axis of plots (Default)
	X-SCALE=INVERSE	Uses inverse scale on horizontal axis of plots
Y-SCALE	**Y-SCALE=STANDARD**	Uses linear scale on vertical axis of plots (Default)
	Y-SCALE=INVERSE	Uses inverse scale on vertical axis of plots
	Y-SCALE=LOG	Uses logarithmic scale on vertical axis of plots
WIDE, GRID, INTERPOLATE	Plot options. Use to override defaults established by the PLOT-OPTIONS paragraph. (See Chapter 46.)	

PT Envelope Tables

Input Language for PT ENVELOPE

```
PROP-TABLE    tableid    PTENVELOPE
DESCRIPTION    "a property table description – up to 64 characters in quotes"
PROPERTIES    opsetname    keyword=value
```

Optional keywords:

FREE-WATER SOLU-WATER HENRY-COMPS CHEMISTRY TRUE-COMPS

```
BLOCK-OPTIONS    keyword=value
```

Optional keywords:

SIM-LEVEL PROP-LEVEL

```
STREAM    sid
basis-FLOW    cid    flow  / . . .
ENVELOPES    VFRAC=value-list
PARAM    keyword=value
```

Optional keywords:

MAXPT PINIT TINIT REDT

TABULATE	**"heading"**	**PROPERTIES=propsetid-list**	*keyword=value*

Optional keywords:

PRINT-PLOT HIGH-PRECISION LINES X-SCALE Y-SCALE WIDE GRID INTERPOLATE

Input Language Description for PT ENVELOPE

tableid ..... Property table ID

DESCRIPTION A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the PROP-TABLE paragraph report.

PROPERTIES Use to replace the flowsheet property specifications. Any option set entered here must also be named in the PROPERTIES paragraph. (See Chapter 8.)

BLOCK-OPTIONS Use to override the diagnostic message levels established by the DIAGNOSTICS paragraph. (See Chapter 45.)

STREAM Use to reference a stream from a simulation. You cannot use the STREAM sentence if you used the basis-FLOW sentence.

sid..... Stream ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

basis-FLOW Use to define mixtures on a MOLE, MASS, or STDVOL basis. You cannot use basis-FLOW if you specified STREAM sentence.

cid..... Component ID

flow ..... Flow rate on a MOLE, MASS, or STDVOL basis

ENVELOPES Use to specify the vapor fraction branches.

VFRAC..... List of vapor fractions. One PT envelope is generated for each value entered. For each vapor fraction specified, the complementary branch is automatically generated.

PARAM Specify either PINIT or TINIT, but not both. If neither is specified, the default is PINIT=1 atm.

MAXPT ..... Maximum number of points (up to 100) along a curve of constant vapor fraction (Default=50)

PINIT..... Pressure at the initial point

TINIT..... Temperature at the initial point

REDT..... Specified value of the mixture reduced temperature at which the calculations are terminated after passing through the mixture critical point (Default=0)

TABULATE Use to specify the properties to be tabulated. You do not need to specify temperature and pressure in a PROP-SET sentence because they are tabulated automatically. You can also use the TABULATE sentence to generate print-plots and to specify plot options.

heading..... String of up to 60 characters, enclosed in quotes

PROPERTIES ..... List of property set IDs for the properties to be tabulated. (See Chapter 41.)

PRINT-PLOT.....	**PRINT-PLOT=YES**	Generates print-plots are generated
	PRINT-PLOT=NO	Does not generate print-plots (Default)
HIGH-PRECISION	**HIGH-PRECISION=YES**	Prints seven significant digits in tables
	HIGH-PRECISION=NO	Prints five significant digits in tables (Default)

LINES	Number of rows of values to print in tables before printing a grid line. If LINES=0, no grid lines are printed. Must be between 0 and 35. (Default=5)	
X-SCALE	**X-SCALE=STANDARD**	Uses linear scale on horizontal axis of plots (Default)
	X-SCALE=INVERSE	Uses inverse scale on horizontal axis of plots
Y-SCALE	**Y-SCALE=STANDARD**	Uses linear scale on vertical axis of plots (Default)
	Y-SCALE=INVERSE	Uses inverse scale on vertical axis of plots
	Y-SCALE=LOG	Uses logarithmic scale on vertical axis of plots
WIDE, GRID, INTERPOLATE	Plot options. Use to override defaults established by the PLOT-OPTIONS paragraph. (See Chapter 46.)	

Residue Curves

Input Language for RESIDUE

```
PROP-TABLE    tableid    RESIDUE
DESCRIPTION    "a property table description – up to 64 characters in quotes"
PROPERTIES    opsetname    keyword=value
```

Optional keywords:

FREE-WATER SOLU-WATER HENRY-COMPS CHEMISTRY TRUE-COMPS

```
BLOCK-OPTIONS    keyword=value
```

Optional keywords:

SIM-LEVEL PROP-LEVEL

```
RESIDUE    COMPS=comp-list
STATE    PRES=pres
PARAM    keyword=value
```

Optional keywords:

MAXIT TOL NGRID NPHASE

Input Language Description for RESIDUE

tableid ..... Property table ID

DESCRIPTION A string of up to 64 characters enclosed in quotes. Aspen Plus prints this description in the header section of the PROP-TABLE paragraph report.

PROPERTIES Use to replace the flowsheet property specifications. Any option set entered here must also be named in the PROPERTIES paragraph. (See Chapter 8.)

BLOCK-OPTIONS Use to override the diagnostic message levels established by the DIAGNOSTICS paragraph. (See Chapter 45.)

RESIDUE Use to define the ternary mixture.

COMPS ..... Component IDs. You must specify three components.

STATE Use to enter pressure specification for the system.

PRES ..... Pressure (Default=1 atm)

PARAM Use to specify optional convergence, grid density and phase specification.

MAXIT ..... Maximum number of flash iterations. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

TOL ..... Flash tolerance. (Default=value established by the SIM-OPTIONS paragraph.) (See Chapter 45.)

NGRID ..... Grid density parameter: LOW, MEDIUM, or HIGH.

NPHASE ..... **NPHASE=2** Two-phase flash (Default)

NPHASE=3 Three-phase flash

41 Defining Property Sets

This chapter describes the input language used for defining property sets and user property set properties.

A property set can be used in:

- Unit operation block heating and cooling curve reports.
- Distillation column stage property reports and performance specifications.
- Design specifications.
- Calculator blocks.
- Optimization.
- Sensitivity and case-study blocks.
- Data-fit.
- Stream reports and report scaling.
- Physical property tables.

Defining Property Sets

Input Language for PROP-SET

PROP-SET	**propsetid**	**propname-list**	*keyword=value*

Optional keywords:

COMPS PHASE BASIS UNITS TEMP PRES LVPCT L2COMPS SUBSTREAM

Input Language Description for PROP-SET

Use the PROP-SET paragraph to define a property set. A property set is a collection of thermodynamic, transport, and other properties. Each property set you define is identified by an ID you supply.

propsetid		Property set ID
propname-list		List of property names. (See *Aspen Plus Physical Property Data*, Tables 4.1 through 4.9.)
COMPS		List of component IDs (applies to all properties listed in *Aspen Plus Physical Property Data*, Tables 4.2 through 4.5, 4.8 and 4.9). (Default=all components actually present when the property is calculated.) (See Note 3.)
PHASE	**PHASE=V**	Vapor
	PHASE=L	Total liquid
	PHASE=L1	First-liquid
	PHASE=L2	Second-liquid
	PHASE=T	Total mixture
	PHASE=S	Solid
		Phase compositions are determined at stream conditions. (See Note 1.) (Default=T, if listed as a valid phase for the property in *Aspen Plus Physical Property Data*, Tables 4.1 through 4.9; otherwise no default.)
BASIS	**BASIS=WET**	Includes water (Default)
	BASIS=DRY	Excludes water
UNITS		Units options selected for the units keywords that are listed for the property in *Aspen Plus Physical Property Data*, Tables 4.1 through 4.9. (Default=IN-UNITS if PROP-SET is specified for design specifications, Calculator blocks, optimization paragraphs and constraint paragraphs. Default=OUT-UNITS if PROP-SET is specified for reports. If a property has mole, mass, or flow units, the default will be mole units.)
TEMP		Temperatures for property calculations. (See Note 2.) (Default=stream temperature. For VVSTD and VVSTDMX, Default=25ºC.)
PRES		Pressures for property calculations. (See Note 2.) (Default=stream pressure. For VVSTD and VVSTDMX, Default=1 atm.)

LVPCT ..... Liquid percents. LVPCT is on a volume basis for *propnames*: TBPT, D86T, D1160T, and VACT. LVPCT is on a weight basis for: TBPWT, D86WT, D1160WT, and VACWT.

L2-COMPS ..... List of key components that identify the second-liquid phase when PHASE=L1 or PHASE=L2, and rigorous three-phase flash calculations are performed. The liquid phase with the larger mole fraction of the key components is designated as the second-liquid phase.

SUBSTREAM ..... Substream ID. (See Notes 3 and 4.) (Default=MIXED)

Defining User PROP-SET Properties

Input Language for USER-PROPERTY

USER-PROPERTY	**userpropid**	**propname**	*keyword=value*

Keyword:

SUBROUTINE

Optional keywords:

FLASH UNIT-TYPE UNIT-LABEL COMP-DEP LVPCT-DEP CURVE-PROP DEFAULT-PROP BLEND-METHOD BLEND-OPT EXTRAPOLATE

Input Language Description for USER-PROPERTY

Use the USER-PROPERTY paragraph to define the property. This property can be referenced in the PROP-SET paragraph in the same way as built-in properties. You must supply a FORTRAN subroutine to calculate the value of the user PROP-SET properties.

userpropid ..... User property ID. This property must be different from built-in properties. (See *Aspen Plus Physical Property Data*, Tables 4.1 through 4.9.)

SUBROUTINE ..... Name of user-supplied subroutine for calculating the property. For details on writing the user-supplied subroutine, see *Aspen Plus User Models*, Chapter 7.

FLASH .....

FLASH=NO	Does not flash the stream before the user-supplied subroutine is called (Default)
FLASH=NOCOMPOSITE	Does not flash the stream for total stream properties (when PHASE=T in the PROP-SET paragraph), but flashes for any other phase specification
FLASH=YES	Always flashes stream before the user-supplied subroutine is called

UNIT-TYPE ..... Units keyword for the property. If not entered, unit conversion is not performed on property values returned from the user-supplied subroutine.

UNIT-LABEL ..... Unit label for the property printed in the report. A unit label is used only when unit conversion is performed by the user-supplied subroutine (that is, when UNIT-TYPE is not given).

COMP-DEP	**COMP-DEP=YES**	Property is a component property
	COMP-DEP=NO	Property is a mixture property (Default)
LVPCT-DEP	**LVPCT-DEP=YES**	Uses liquid percent in calculating the property. The combination COMP-DEP=YES and LVPCT-DEP=YES is not allowed for the same property.
	LVPCT-DEP=NO	Does not use liquid percent in calculating the property (Default)
CURVE-PROP	**CURVE-PROP=YES**	Defines a property to be a petroleum assay curve property. You can enter curve data for a petroleum assay property in the ASSAY/BLEND paragraphs. (See Chapter 7.)
	CURVE-PROP=NO	Does not define a property curve (Default)

DEFAULT-PROP Default property name for real components when CURVE-PROP=YES. The pure component property provides default values for light-ends components. (See *Aspen Plus Physical Property Methods and Models*, Chapter 3.)

BLEND-METHOD Blending option for the petroleum assay curve property. The blending option is used in two ways: to generate property curves for blends from assay curves, and to compute stream properties by blending individual pseudocomponent property values.

BLEND-METHOD=MOLE	Mole fraction averaging
BLEND-METHOD=MASS	Mass fraction averaging
BLEND-METHOD=STDVOL	Standard-liquid-volume averaging (Default)
BLEND-METHOD=USER	Uses a user-supplied subroutine (BLDPPU) for blending. For details on writing a user-supplied subroutine, see *Aspen Plus User Models*, Chapter 9.

BLEND-OPTION Blending option code for user-supplied blending routine, when you specify BLEND-METHOD=USER. The option code is passed as an argument to the user-supplied blending subroutine BLDPPU. This option allows you to implement multiple user blending methods, within the same subroutine. For details on writing a user-supplied subroutine, see *Aspen Plus User Models*, Chapter 9.

EXTRAPOLATE	**EXTRAPOLATE=YES**	Extrapolates curve data if it does not encompass the 0% and 100% points (Default)
	EXTRAPOLATE=NO	Does not extrapolate curve data

Notes

1 The phases selected should be consistent with the application. For example, if first-liquid and second-liquid phase properties are requested for a HEATER heating/cooling curve, then the HEATER block must perform either rigorous three-phase or free-water calculations. When a stream property is requested, the stream is flashed according to flash options established by the STREAM paragraph or source block for the stream.

2 The TEMP and PRES qualifiers are used to evaluate properties at temperatures and pressures that differ from those of the stream. However, TEMP and PRES have no effect on the compositions of vapor and liquid phases. These compositions are determined at the stream temperature and pressure.

3 When a conventional solid substream is present, COMPS should be used with both MIXED and solid substream properties, to list the components actually present in those substreams.

4 To obtain a conventional solid property, both PHASE=S and a conventional solid substream ID must be specified. To obtain a nonconventional solid property, both PHASE=S and a nonconventional solid substream ID must be specified.

42 Regressing Property Data

This chapter describes the input language for performing property data regression. The paragraphs are:

Use this paragraph	To
PARAMETERS	Define property parameters to be used in regression
DATA-GROUP	Enter experimental data or generate vapor-liquid or liquid-liquid equilibrium data
CASE	Specify parameters, data groups, option sets, and algorithm parameters for regression cases
TABULATE	Generate property tables and plots

PARAMETERS Paragraph

Input Language for PARAMETERS

```
PARAMETERS
PARAMETER paramno paramname cid elemno [initial] [lower] &
      [upper] [scale]
BIPARAMETER paramno paramname cid1 cid2 elemno [initial] &
      [lower] [upper] [scale]
SBIPARAMETER paramno paramname cid1 cid2 elemno [initial] &
      [lower] [upper] [scale]
GROUP-PARAM paramno paramname gid setno [initial] [lower] &
      [upper] [scale]
GROUP-BIPARAM paramno paramname gid1 gid2 setno [initial] &
      [lower] [upper] [scale]
PAIRPARAMETER paramno paramname pair1 pair2 elemno [initial] &
      [lower] [upper] [scale]
K-SALT paramno chemid saltid coefno [initial] [lower] [upper] &
      [scale]
K-STOIC paramno chemid reacno coefno [initial] [lower] &
      [upper] [scale]
```

Input Language Description for PARAMETERS

PARAMETER, BIPARAMETER, SBIPARAMETER GROUP-PARAM, GROUP-BIPARAM, PAIRPARAMETER, K-SALT, K-STOIC

Defines parameters to be used in the regression. Use to enter optional initial estimates, lower and upper bounds, and scale factors. Use GROUP-PARAM and GROUP-BIPARAM for UNIFAC group parameters. Use PAIRPARAMETER for the electrolyte NRTL model. Use K-SALT and K-STOIC for the equilibrium constants of salt precipitation and chemical equilibrium reactions. Use SBIPARAMETER to force unsymmetric binary parameters (such as NRTL a_{ij}) to be symmetric during the regression (for example, use it to regress values for NTRL a_{ij} but set $a_{ij} = a_{ji}$).

paramno ..... Parameter number. An integer number you assign, which is used to reference the parameters in the CASE paragraph.

paramname ..... Parameter name. Must be the parameter of an option set listed in the PROPERTIES paragraph. Parameter names associated with Aspen Plus physical property models are listed in *Aspen Plus Physical Property Methods and Models*, Chapter 3. TABPOLY model parameter names are listed in Chapter 8. Aspen Plus user-model parameter names are listed in *Aspen Plus User Models*, Chapter 6. For the generic user property Y, the parameter name is GENPRP. For the general user property, you can use the parameter names DRUSR1 and DRUSR2. You can also use any parameters you defined using the USER-PROPS paragraph. (See Chapter 8.)

cid, cid1, cid2..... Component ID. For asymmetric binary parameters, use *cid1 cid2* for the first parameter and *cid2 cid1* for the second parameter. For symmetric binary parameters, use either *cid1 cid2* or *cid2 cid1*.

elemno..... Parameter element number (Default=1)

initial ..... Optional initial estimate of the parameter. Must be in SI units.

lower ..... Optional lower bound of the parameter. Must be in SI units.

upper ..... Optional upper bound of the parameter. Must be in SI units.

scale	Optional multiplier to scale the numerical magnitude of a parameter. Recommended value is the reciprocal of a typical value for the parameter. (Default=1)
gid, gid1, gid2	UNIFAC group ID, as defined in the GROUPS paragraph. (See Chapter 8.) UNIFAC group binary parameters are asymmetric. Use *gid1 gid2* for the first parameter and *gid2 gid1* for the second parameter. You can regress only the first element of the UNIFLB and UNIFDM parameters.
setno	Data set number. For option set UNIFAC use *setno*=1. For option set UNIF-LL use *setno*=2.
pair1, pair2	Component IDs for component pair. For electrolyte, *pair*=cation anion. For molecular species, *pair*=cid.
chemid	Chemistry ID for CHEMISTRY paragraph
saltid	Salt ID from a K-SALT sentence in the CHEMISTRY paragraph
reacno	Equilibrium reaction number from a K-STOIC sentence in the CHEMISTRY paragraph
coeffno	Coefficient number in the equilibrium constant expression for K-SALT and K-STOIC ln (K) = a + b/T + c ln T + dT Where *coeffno* = 1 for *a*, *coeffno* = 2 for *b*, and so on

DATA-GROUP Paragraph

Input Language for DATA-GROUP

To enter experimental data:

```
DATA-GROUP    dataid
IN–UNITS    set    keyword=option
DESCRIPTION    "a data-group description - up to 64 characters long"
SYSTEM–DEF    statespec    cid–list    [PROP–LIST=proplist]    &
      [COMPOSITION=option]
PHASE–EQ    peqtype    cid–list  /  ...
CHEM-EQ    SALT    saltid-list
DATA    datano    value-list  /  ...
STD–DEV    std–devno    value–list  /  ...
```

To generate VLE or LLE data:

```
DATA-GROUP    dataid
IN-UNITS    set    keyword=option
DESCRIPTION    "a data-group description - up to 64 characters long"
GENERATE    statespec    cid1    cid2    opsetname    keyword=value
```

Optional keywords:

HENRY-COMPS   TEMP   PRES   MOLE-FRAC

Input Language Description for DATA-GROUP

dataid ..... Data group ID

IN-UNITS Input units for measurement data. (See Chapter 3.)

set ..... ENG, SI, or MET (Default=ENG)

keyword..... Units keyword. (See Chapter 3.)

option ..... Units option. See Chapter 3. This specification overrides the corresponding units option contained in the specified set.

DESCRIPTION Description printed in the report file, when reporting the results of the data group. Aspen Plus uses the description as a label for the experimental data, in print-plots, and in the plot file.

SYSTEM-DEF Use to define the state and property variables, component IDs, and types of composition data.

statespec ..... State variables. Tables 43.1 through 43.4 provide valid options for various types of data.

cid-list ..... List of component IDs. The order of the components specifies the order of the composition data and partial properties to be entered in DATA sentences. For pure component properties (see Table 43.1), list only one component.

PROP-LIST ..... List of properties. Omit this list when all measured variables are state variables, such as for VLE data. Tables 43.1 through 43.3 list valid property specifications.

COMPOSITION ..... Type of composition data:

COMPOSITION= MOLE–FRAC	Mole fraction (Default)
COMPOSITION= MASS–FRAC	Mass fraction
COMPOSITION= MOLE–PERCENT	Mole percent
COMPOSITION= WEIGHT-PERCENT	Weight percent

PHASE-EQ Use to specify the type of phase equilibrium (such as vapor-liquid or liquid-liquid), and the components that must satisfy the phase equilibrium constraints. By default DRS automatically determines the type of phase equilibrium and the components involved from the state specification you made in the SYSTEM-DEF sentence. You can use the optional PHASE-EQ sentence to override the default phase equilibrium type, or to specify a smaller number of components that must satisfy the phase-equilibrium constraints when the mixture contains non-volatile components, such as ions or high-boiling compounds.

peqtype ..... Phase equilibrium type. See Table 43.5 for valid options.

cid-list ..... List of components for which phase equilibrium is satisfied. Can be a subset of the list specified in the SYSTEM-DEF sentence, when the mixture contains non-volatile components.

CHEM-EQ Use to specify chemical equilibrium constraints for salt precipitation. Use with salt solubility data.

saltid-list ..... List of salt IDs obtained from CHEMISTRY paragraphs for precipitating salt components.

DATA Use to enter measurement data. Enter the data in the same order as the list of state variables, properties, and components specified in the SYSTEM-DEF sentence.

datano ..... Data point number

value-list ..... List of measured values. Use an asterisk (*) for a missing composition data value (such as a missing Y from *statespec* is TPXY). An asterisk for a missing property measurement, such as PL, removes this measurement from the regression.

STD-DEV

Use to enter the optional standard deviations of measured variables for all data points. The number of standard deviation values in each STD-DEV sentence equals the number of measurement values in the DATA sentence.

std-devno ..... Standard deviation number, corresponding to the ordinal data point number

value-list ..... List of standard deviations. Use an asterisk (*) for the standard deviation of a missing state variable or property.

GENERATE

Use to specify the type of phase-equilibrium data to be generated, the components, the property option set to be used, and the temperature, pressure, and compositions at which the data are to be generated. Use GENERATE only for binary systems.

statespec ..... **TPXY** Generates VLE data

TPXX Generates LLE data

cid1, cid2 ..... IDs for the two components

opsetname..... Name of the property option set used to generate the binary VLE or LLE data. Cannot be the same as the option set used in the CASE paragraph that references this data group. (Default=the first option set listed in the PROPERTIES paragraph.)

HENRY-COMPS..... Henry's constant component list ID

TEMP..... List of temperature values:
If *statespec* is TPXY, you can specify either TEMP or PRES, but not both. If you do not specify either one, PRES=1 atm is used.
If *statespec* is TPXX, you can specify TEMP (Default=25°C).

PRES..... List of pressure values (Default=1 atm)
If *statespec* is TPXY, you can specify either TEMP or PRES, but not both. If you do not specify either one, PRES=1 atm is used.

MOLE-FRAC..... List of mole-fraction values:
Default =

0.01	0.05	0.10	0.15	0.20	0.25	0.30
0.35	0.40	0.45	0.50	0.55	0.60	0.65
0.70	0.75	0.80	0.85	0.90	0.95	0.99

Table 43.1 Pure Component Properties

Property Name	Description	Valid State Specifications
CPL	Liquid molar heat capacity	T, TP
CPS	Solid molar heat capacity	T, TP
CPV	Vapor molar heat capacity	T, TP
DHLS	Molar enthalpy of transition (L-S)	T, TP
DHVL	Molar enthalpy of vaporization (V-L)	T, TP
DHVS	Molar enthalpy of sublimation (V-S)	T, TP
HL	Liquid molar enthalpy	T, TP
HS	Solid molar enthalpy	T, TP
HV	Vapor molar enthalpy	T, TP
KL	Liquid thermal conductivity	T, TP
KS	Solid thermal conductivity	T, TP
KV	Vapor thermal conductivity	T, TP
MUL	Liquid viscosity	T, TP
MUV	Vapor viscosity	T, TP
PL	Liquid vapor pressure	T
PS	Solid vapor pressure	T
RHOL	Liquid mass density	T, TP
RHOS	Solid mass density	T, TP
RHOV	Vapor mass density	T, TP
SIGL	Surface tension	T, TP
USER	User property	T, TP
VL	Liquid molar volume	T, TP
VS	Solid molar volume	T, TP
VV	Vapor molar volume	T, TP
WATSOL	Water solubility	T, TP
Y	Generic property	T

Table 43.2 Mixture Properties

Property Name	Description	Valid State Specifications†
CPLMX	Liquid molar heat capacity	TX, TPX
CPVMX	Vapor molar heat capacity	TY, TPY
GAMMAM	Mean activity coefficient	TX, TPX
GLXS	Liquid molar excess free energy	TX, TPX
HLMX	Liquid molar enthalpy	TX, TPX
HLXS	Liquid molar excess enthalpy	TX, TPX
HVMX	Vapor molar enthalpy	TY, TPY
KLMX	Liquid thermal conductivity	TX, TPX
KVMX	Vapor thermal conductivity	TY, TPY
MULMX	Liquid viscosity	TX, TPX
MUVMX	Vapor viscosity	TY, TPY
OSMOT	Osmotic coefficient	TX, TPX
PH	pH	TX, TPX
RHOLMX	Liquid mass density	TX, TPX
RHOVMX	Vapor mass density	TY, TPY
SIGLMX	Surface tension	TX, TPX
USERMX	User property	TX, TPX, TY, TPY
VLMX	Liquid molar volume	TX, TPX
VVMX	Vapor molar volume	TY, TPY

† For TX or TY specifications, DRS assumes P=1 bar.

Table 43.3 Component (Partial) Properties in Mixtures

Property Name†	Description	Valid State Specifications††
DLMX	Liquid diffusion coefficient	TX, TPX
DVMX	Vapor diffusion coefficient	TY, TPY
GAMMA	Liquid activity coefficient	TX, TPX
GAMMAS	Solid activity coefficient	TX, TPX
HNRYMX	Henry's constant	TX, TPX
KLL	Liquid-liquid distribution coefficient	TXX, TPXX
KVL	Vapor-liquid K-value	TXY, TPXY
USERI	User property	TX, TPX, TY, TPY

† You must enter property values for all components.

†† For TX or TY specifications, DRS assumes P=1 bar.

Table 43.4 State Specifications for Phase Equilibrium Data

Type of Phase Equilibrium Data	Valid State Specifications
Vapor-liquid†	TXY, TPXY
Liquid-liquid††	TXX, TPXX
Vapor-liquid-liquid†††	TXXY, TPXXY
Vapor-liquid†††	TP
Salt solubility	TX, TPX, TPXY

† For TXY specification, DRS estimates the value of P, assigns a large standard deviation value for P, and includes it in the regression.

†† For TXX and TXXY specifications, DRS assumes P=1 bar.

††† Pure component vapor pressure data are VLE data. Two types of regressions use vapor pressure data: regression of the extended Antoine vapor pressure equation; and regression of equation-of-state parameters, such as eccentric factor and polar parameters for pure components. In the first case, the state specification is T and the property is PL. In the second case, the state specification is TP and there is no property.

Table 43.5 Phase Equilibrium Specifications for PHASE-EQ Sentence

Type of Phase Equilibrium Data	Peqtype Specification
Vapor-liquid	VL
Liquid-liquid	LL
Vapor-liquid-liquid†	Any two of VL1, VL2, and LL

† Use two PHASE-EQ sentences. For example: PHASE-EQ VL1 cid-list / LL cid-list.

CASE Paragraph

Input Language for CASE

```
CASE    caseid
CASE-OPTION    keyword=value
```

Optional keywords:

REGRESSION OBJECT-FUNC SIM-LEVEL PROP-LEVEL LL-TEST FORM

```
PARAMETERS    keyword=value-list
```

Keywords:

PURE BINARY GROUP-PURE GROUP-BINARY PAIR K-SALT K-STOIC

```
DATA-GROUPS    dataid    keyword=value  / ...
```

Optional keywords:

WEIGHT CONSISTENCY METHOD REJECT AREA-TOL POINT-TOL

```
PROPERTIES    opsetname    keyword=value
```

Optional keywords:

HENRY-COMPS CHEMISTRY TRUE-COMPS

```
ALGORITHM    keyword=value
```

Optional keywords:

MAXIT INIT-MAXIT ZLOOP-MAXIT TOL METHOD INIT-METHOD BRITT-LUECKE STEPSIZE NUM-DERIV SSND ONE-D-SEARCH

```
INIT-PARAM    paramno    keyword=value  / ...
```

Keywords:

CASE VALUE

```
SET-PARAM    paramname    cid    elemno    value
SET-BIPARAM    paramname    cid1    cid2    elemno    value
SET-GPARAM    paramname    gid    setno    value
SET-GBPARAM    paramname    gid1    gid2    setno    value
REPORT    reportopt-list
```

Report options:

KVL GAMMA TBUB PBUB TXX KLL

Input Language Description for CASE

caseid ..... Case ID

CASE-OPTION

Use to specify whether to perform a regression, override the default objective function, control the regression and property diagnostic message level, and select the form of the built-in equation for generic property Y.

REGRESSION..... REGRESSION=YES Performs regression (Default)

	REGRESSION=NO	Does not perform regression. Evaluates property model parameters using the input parameters and the data groups specified, or test the binary VLE data for thermodynamic consistency.

OBJECT-FUNC..... Specify the objective function in VLE regression:

OBJECT-FUNC=ML	Maximum likelihood (Default)
OBJECT-FUNC=OLS	Ordinary least squares. P and Y are dependent variables for isothermal data. T and Y are dependent variables for isobaric data.
OBJECT-FUNC=PY	Modified Barker's method. P and Y are dependent variables.
OBJECT-FUNC=BARKER	Barker's method. P is dependent variable.
OBJECT-FUNC=GAMMA	Activity coefficients are dependent variables. DRS calculates experimental activity coefficients from VLE (TPXY) data.
OBJECT-FUNC=KVL	K-values are dependent variables. DRS calculates experimental K-values from VLE (TPXY) data.
OBJECT-FUNC=ALPHA	Relative volatility. Defined relative to the first component.

SIM-LEVEL ..... Override the global regression message level. (Default=value established in the DIAGNOSTICS paragraph.) (See Chapter 45.)

PROP-LEVEL..... Override the global property message level. (Default=value established in the DIAGNOSTICS paragraph.) (See Chapter 45.)

LL-TEST..... Test correctness of LLE results at the end of DRS by performing phase stability test.

LL-TEST=YES	Performs the test (Default)
LL-TEST=NO	Does not perform the test

FORM ..... Form of the built-in equation used in fitting the generic property *Y*. See the DATA-GROUP paragraph for information on how to enter generic data.

FORM=NORMAL Use the following equation: (Default)

$$Y = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 + a_6 T^{1/2} + a_7 / T + a_8 / T^2 + a_9 / T^3 + a_{10} / T^4 + a_{11} / T^{1/2} + a_{12} \ln(T)$$

FORM=LOG Use the following equation:

$$\ln Y = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 + a_6 T^{1/2} + a_7 / T + a_8 / T^2 + a_9 / T^3 + a_{10} / T^4 + a_{11} / T^{1/2} + a_{12} \ln(T)$$

PARAMETERS Use to specify the parameters to be regressed. The parameters must already be defined in the PARAMETERS paragraph.

PURE..... List of pure component parameter numbers for parameters to be regressed in this case. Parameter numbers are defined in the PARAMETER sentences.

BINARY..... List of binary parameter numbers for parameters to be regressed in this case. Parameter numbers are defined in the BIPARAMETER sentences.

GROUP-PURE ..... List of UNIFAC group parameter numbers for parameters to be regressed in this case. Parameter numbers are defined in the GROUP-PARAM sentences.

GROUP-BINARY ..... List of UNIFAC group binary parameter numbers for parameters to be regressed in this case. Parameter numbers are defined in the GROUP-BIPARAM sentences.

PAIR ..... List of electrolyte NRTL pair parameter numbers for parameters to be regressed in this case. Parameter numbers are defined in the PAIRPARAMETER sentences.

K-SALT ..... List of K-SALT ID numbers for parameters to be regressed in this case. Parameter numbers are defined in the K-SALT sentences.

K-STOIC ..... List of K-STOIC ID numbers for parameters to be regressed in this case. Parameter numbers are defined in the K-STOIC sentences.

DATA-GROUPS

Use to select experimental data to be used. The data groups must already be defined in a DATA-GROUP paragraph.

dataid ..... Data group ID

WEIGHT ..... Relative weight of the data (Default=1)

CONSISTENCY ..... **CONSISTENCY=YES** Tests binary VLE data for thermodynamic consistency

CONSISTENCY=NO Does not test binary VLE data for thermodynamic consistency (Default)

METHOD ..... Method to test binary VLE data for thermodynamic consistency:

METHOD=AREA Area test (Default)

METHOD=POINT Point test

METHOD=BOTH Both methods

REJECT ..... **REJECT=YES** Does not use inconsistent data in this regression

REJECT=NO Uses inconsistent data in this regression (Default)

AREA-TOL ..... Tolerance for the area test (Default=10%)

POINT-TOL ..... Tolerance for the point test. POINT-TOL is not allowed when METHOD=AREA. (Default=0.01)

PROPERTIES

Use to specify the property option set. The default is the global property specification in the PROPERTIES paragraph. You must name any option set that you enter here in the PROPERTIES paragraph.

opsetname ..... Option set name

HENRY-COMPS ..... Henry's component list ID

CHEMISTRY ..... Chemistry ID

TRUE-COMPS ..... True or apparent component approach. Use in electrolytes:

TRUE-COMPS=YES True component approach (Default)

TRUE-COMPS=NO Apparent component approach

ALGORITHM

Use to specify parameters for the regression algorithm.

MAXIT ..... Maximum number of iterations (Default=50)

INIT-MAXIT ..... Maximum number of iterations during the initialization step (Default=20)

ZLOOP-MAXIT ..... Maximum number of iterations during the measurement variable adjustment step, after the initialization step (Default=10)

TOL ..... Convergence tolerance (Default=1×10^{-4})

METHOD ..... **METHOD=NEW** New regression method (Default)

		METHOD=OLD	Old algorithm
	INIT-METHOD	Method used in the initialization step:	
		INIT-METHOD=DEMING	Deming method (Default)
		INIT-METHOD=WLS	Weighted least squares
	BRITT-LUECKE	**BRITT-LUECKE=YES**	Uses Britt-Luecke algorithm, after the initialization step (Default)
		BRITT-LUECKE=NO	Does not use Britt-Luecke algorithm
	STEPSIZE	Maximum step size of parameter adjustments (Default=0.1)	
	NUM-DERIV	**NUM-DERIV=FORWARD**	Uses the forward difference method to compute the numerical derivative (Default)
		NUM-DERIV=CENTRAL	Uses the central difference method to compute the numerical derivative
	SSND	Step size used to calculate numerical derivative. (Default=$1x10^{-4}$)	
	ONE-D-SEARCH	One-dimensional search key. Use when METHOD=OLD:	
		ONE-D-SEARCH=YES	Performs one-dimensional search during the Deming iterations (Default)
		ONE-D-SEARCH=NO	Does not perform one-dimensional search
INIT-PARAM	Use to assign initial estimates for regression parameters in the current case. The value replaces, for this case, the initial estimate entered in the PARAMETERS paragraph. You can either enter a value or use results from any preceding case, but you cannot do both.		
	paramno	Parameter number for regression parameter you want to initialize for this case	
	CASE	Case ID. Uses results from the case specified to initialize the parameter. The case specified must precede the current case.	
	VALUE	Numerical value assigned to the parameter as initial guess	
SET-PARAM, SET-BIPARAM	Use to assign a numerical value for pure component and binary parameters that are not being regressed in this case.		
	paramname	Parameter name	
	cid, cid1, cid2	Component IDs	
	elemno	Parameter element number	
	value	Numerical value assigned to the parameter	
SET-GPARAM, SET-GBPARAM	Use to assign a numerical value to UNIFAC group and group binary parameters that are not being regressed in this case.		
	paramname	Parameter name	
	gid, gid1, gid2	Group IDs	
	setno	Data set number. Uses *setno*=1 when option set UNIFAC is specified. Uses *setno*=2 for UNIF-LL.	
	value	Numerical value assigned to the parameter	
REPORT	Use to specify additional properties to be printed in the report file.		
	KVL	Vapor-liquid K-values	
	GAMMA	Liquid activity coefficients	
	TBUB	Bubble point temperature. DRS performs bubble-point temperature (PV) flashes at the experimental pressures and liquid compositions. Calculated vapor compositions are also reported.	

PBUB..... Bubble point pressure. DRS performs bubble-point pressure (TV) flashes at the experimental temperatures and liquid compositions. Calculated vapor compositions are also reported.

TXX..... Liquid-liquid coexistence curve. DRS performs three-phase TP flashes at the experimental temperatures, pressures, and overall liquid compositions. The calculated compositions for both liquid phases are reported.

KLL..... Liquid-liquid distribution coefficients

TABULATE Paragraph

Input Language for TABULATE

TABULATE
PROPERTY **propno** **"heading"** *keyword=value*

Keywords:

PROPS **X-AXIS** **COMP** **DATA** **DATA-GROUPS** **CASE**

Optional keywords:

HIGH-PRECISION **LINES** **X-SCALE** **Y-SCALE** **WIDE** **GRID** **INTERPOLATE** **PRINT-TABLE** **PRINT-PLOT** **PLOT-FILE**

ERROR **errorno** **"heading"** *keyword=value*

Keywords:

PROPS **X-AXIS** **COMP** **CASE**

Optional keywords:

HIGH-PRECISION **LINES** **X-SCALE** **Y-SCALE** **WIDE** **GRID** **INTERPOLATE** **PRINT-TABLE** **PRINT-PLOT** **PLOT-FILE**

Input Language Description for TABULATE

PROPERTY Use for tabulating experimental data and/or regression results. Use to specify properties and components to be tabulated, variables for the x-axis, and whether experimental data will be included. Also use to specify data groups to be used, cases from which the calculated results will be obtained, and options for the tabulation.

propno..... Property tabulation number. Must be an integer value.

heading..... Heading up to 64 characters enclosed in quotes

ERROR Use for tabulating property errors. Use to specify properties, variables for the x-axis, and components to be tabulated. Also use to specify cases from which the calculated results will be obtained, and options for the tabulation.
The error or deviation is defined as: calculated value – experimental value.

errorno..... Error tabulation number. Must be an integer.

heading..... Heading up to 64 characters enclosed in quotes

PROPS		List of properties (or property errors) to be tabulated. Each property will appear on a separate table, print-plot, or section of the plot file. Table 43.6 lists the valid properties. If you specify X, Y, Y*X, or a partial property, you must also specify COMP. Table 43.7 lists common specifications that are useful for analyzing regression results involving VLE and LLE data.
X-AXIS		List of independent variables against which the property is to be tabulated. The valid independent variables are the state variables and the property itself. The number of generated tables, print-plots, or sections in the plot file equals the number of PROPS specified times the number of X-AXIS specified. If you select X, Y, XY, XX, or partial property, you must also specify COMP.
	X-AXIS=TEMP	Temperature
	X-AXIS=PRES	Pressure
	X-AXIS=X	Liquid composition
	X-AXIS=Y	Vapor composition
	X-AXIS=XY	Liquid and vapor compositions. Use for tabulating temperature or pressure versus vapor and liquid compositions, for VLE data.
	X-AXIS=XX	Compositions in both liquid phases. Use for tabulating temperature or pressure versus the compositions of both liquid phases, for LLE data.
	X-AXIS=property	Property itself. Experimental values of the property are tabulated on the X-AXIS.
COMP		Component to be tabulated. If you selected X, Y, XY, XX, or partial property as your X-AXIS, or X, Y, Y*X, or partial property as your PROPS, you must also specify COMP. (Default=most volatile component.)
DATA	**DATA=YES**	Tabulates experimental data. DRS tabulates experimental data from the data groups specified with the DATA-GROUPS keyword and the data groups used in the cases specified with the CASE keyword. (Default)
	DATA=NO	Does not tabulate experimental data
DATA-GROUPS		List of data group IDs. Tabulate experimental data from data groups. Use with DATA=YES.
CASE		List of case IDs. Tabulate calculated results obtained from these cases. If DATA=YES, experimental data are also tabulated. If you want to tabulate only the experimental data, do not use CASE. Instead list the data groups using DATA-GROUPS, and use DATA=YES.
HIGH-PRECISION	**HIGH-PRECISION=YES**	Prints seven significant digits in tables
	HIGH-PRECISION=NO	Prints five significant digits in tables (Default)
LINES		Number of rows of values to print in tables before printing a grid line. If LINES=0, no grid lines are printed. Must be between 0 and 35.
X-SCALE	**X-SCALE=STANDARD**	Uses linear scale on horizontal axis of plots. (Default)
	X-SCALE=INVERSE	Uses inverse scale on horizontal axis of plots
Y-SCALE	**Y-SCALE=STANDARD**	Uses linear scale on vertical axis of plots (Default)
	Y-SCALE=INVERSE	Uses inverse scale on vertical axis of plots
	Y-SCALE=LOG	Uses logarithmic scale on vertical axis of plots

WIDE, GRID, INTERPOLATE	Plot options. Use to override defaults established by the PLOT-OPTIONS paragraph. (See Chapter 46.)	
PRINT-TABLE	**PRINT-TABLE=YES**	Generates tables in the report file (Default)
	PRINT-TABLE=NO	Does not generate tables
PRINT-PLOT	**PRINT-PLOT=YES**	Generates print-plots in the report file (Default)
	PRINT-PLOT=NO	Does not generate print-plots
PLOT-FILE	**PLOT-FILE=YES**	Generates a plot file (Default)
	PLOT-FILE=NO	Does not generate a plot file

Table 43.6 Valid Properties for Tabulation

State Variable:

Property	Description	Valid X-AXIS
PRES	Pressure	TEMP, PRES, X, Y, XY, XX
TEMP	Temperature	TEMP, PRES, X, Y, XY, XX
X	Liquid composition	TEMP, PRES, X, Y
Y	Vapor composition	TEMP, PRES, X, Y
Y*X	Product of vapor and liquid composition	TEMP, PRES, X, Y

Pure Component Properties:

Property	Description	Valid X-AXIS†
CPL	Liquid molar heat capacity	TEMP, PRES
CPS	Solid molar heat capacity	TEMP, PRES
CPV	Vapor molar heat capacity	TEMP, PRES
DHLS	Molar enthalpy of transition	TEMP, PRES
DHVL	Molar enthalpy of vaporization	TEMP, PRES
DHVS	Molar enthalpy of sublimation	TEMP, PRES
HL	Liquid molar enthalpy	TEMP, PRES
HS	Solid molar enthalpy	TEMP, PRES
HV	Vapor molar enthalpy	TEMP, PRES
KL	Liquid thermal conductivity	TEMP, PRES
KS	Solid thermal conductivity	TEMP, PRES
KV	Vapor thermal conductivity	TEMP, PRES
MUL	Liquid viscosity	TEMP, PRES
MUV	Vapor viscosity	TEMP, PRES
PL	Liquid-vapor pressure	TEMP, PRES
PS	Solid-vapor pressure	TEMP, PRES
RHOL	Liquid mass density	TEMP, PRES
RHOS	Solid mass density	TEMP, PRES
RHOV	Vapor mass density	TEMP, PRES
SIGL	Liquid surface tension	TEMP, PRES
USER	User property	TEMP, PRES
VL	Liquid molar volume	TEMP, PRES
VS	Solid molar volume	TEMP, PRES
VV	Vapor molar volume	TEMP, PRES
WATSOL	Water solubility	TEMP, PRES
Y	Generic property	TEMP

† The property itself is a valid X-AXIS specification.

continued

Table 43.6 Valid Properties for Tabulation (continued)

Partial Property:

Property	Description	Valid X-AXIS†
DLMX	Liquid diffusion coefficient	TEMP, PRES, X
DVMX	Vapor diffusion coefficient	TEMP, PRES, Y
GAMMA	Liquid activity coefficient for all components	TEMP, PRES, X
GAMRATIO	Natural logarithm of activity coefficient ratio	TEMP, PRES, X
HNRYMX	Henry's constant	TEMP, PRES, X
KLL	Liquid-liquid distribution coefficient for all components	TEMP, PRES, X
KVL	K-values for all components	TEMP, PRES, X, Y
PHILMX	Liquid fugacity coefficient	TEMP, PRES, X
PHIVMX	Vapor fugacity coefficient	TEMP, PRES, Y
USERI	User property	TEMP, PRES, X, Y

Mixture Properties:

Property	Description	Valid X-AXIS†
CPLMX	Liquid molar heat capacity	TEMP, PRES, X
CPVMX	Vapor molar heat capacity	TEMP, PRES, Y
DGMIX	Total Gibbs free energy of mixing	TEMP, PRES, X
DGMIXRT	Total Gibbs free energy of mixing/RT††	TEMP, PRES, X
GAMMAM	Mean activity coefficient	TEMP, PRES, X
GLXS	Excess Gibbs free energy	TEMP, PRES, X
GLXSRT	Excess Gibbs free energy/RT††	TEMP, PRES, X
HLMX	Liquid molar enthalpy	TEMP, PRES, X
HLXS	Excess enthalpy	TEMP, PRES, X
HLXSRT	Excess enthalpy/RT††	TEMP, PRES, X
HVMX	Vapor molar enthalpy	TEMP, PRES, Y
KLMX	Liquid thermal conductivity	TEMP, PRES, X
KVMX	Vapor thermal conductivity	TEMP, PRES, Y
MULMX	Liquid viscosity	TEMP, PRES, X
MUVMX	Vapor viscosity	TEMP, PRES, Y
OSMOT	Osmotic coefficient	TEMP, PRES, X
PH	pH	TEMP, PRES, X
RHOLMX	Liquid mass density	TEMP, PRES, X
RHOVMX	Vapor mass density	TEMP, PRES, Y
SIGLMX	Liquid surface tension	TEMP, PRES, X
SLXS	Excess entropy	TEMP, PRES, X
SLXSR	Excess entropy/R††	TEMP, PRES, X
USERMX	User property	TEMP, PRES, X, Y
VLMX	Liquid molar volume	TEMP, PRES, X
VSMX	Solid molar volume	TEMP, PRES, X
VVMX	Vapor molar volume	TEMP, PRES, Y

† The property itself is a valid X-AXIS specification.

†† R = Gas constant.

Table 43.7 Common Specifications in VLE or LLE Regression

Property	X-Axis	Description
GAMMA	X	Activity coefficient for all components, versus liquid composition
GAMRATIO	X	Natural logarithm of activity coefficient ratio versus liquid composition
PRES	XY	Pressure versus liquid and vapor compositions for isothermal VLE data
TEMP	XY	Temperature versus liquid and vapor compositions for isobaric VLE data
TEMP	XX	Temperature versus liquid compositions, for both liquid phases, for LLE data
Y	X	Vapor composition versus liquid composition
Y*X	X	Product of vapor and liquid compositions versus liquid composition

43 Stream Libraries

This chapter describes the input language for using the Aspen Plus stream library capability. The Aspen Plus stream library lets you access existing information about stream composition and conditions from a stream library, instead of entering this data in the STREAM paragraph. You can also create your own stream library, or you can use one created and maintained by your Aspen Plus System Administrator.

With the stream library capability, you can:

- Create a library of frequently used feed streams.
- Transfer stream information from one simulation to another.
- Initialize tear streams.
- Isolate a block from a large flowsheet.

To create and use a stream library, you must:

- Create the stream library using the STRLIB program.
- Use the STREAM-LIB paragraph in your Aspen Plus input file to specify which streams you want to retrieve from the library.
- Reference the stream library for an Aspen Plus run.

Creating or Modifying a Stream Library with STRLIB

You can create or modify a stream library using the STRLIB program delivered with Aspen Plus. Every Aspen Plus run produces a summary file that contains all the results of the simulation. The STRLIB program copies stream results from an Aspen Plus summary file into a stream library. You can store data from any number of Aspen Plus runs in one stream library.

Streams in a stream library are organized into cases. You identify a stream by the stream name and the case to which it belongs. Usually, each case corresponds to one Aspen Plus run. However, you can store streams from more than one Aspen Plus run in a single case. You can also store data from a single run in several cases.

STRLIB Commands

You can use STRLIB commands to create or modify a stream library. See Table 44.1 and Description of STRLIB Commands, this chapter, for information about all STRLIB commands. To view a menu of all available commands, type a question mark (?) at the **STRLIB>** prompt. To get online help for these commands, type HELP.

Table 44.1 STRLIB Commands

Command	Description
ADD	Add a stream to the library.
CASE	Change the current case.
DELCASE	Delete a case from the library.
DELSTREAM	Delete a stream from the library.
DIRECTORY	List the cases in the library and the streams in a case.
DUMP	Write stream information to a file.
END	End STRLIB and update the library.
EXIT	End STRLIB and update the library.
HELP	Display interactive help on STRLIB commands.
INITIALIZE	Initialize a library.
LIST	List streams in the summary file.
LOAD	Load stream information from a dump file.
OPEN	Open a summary file.
PACK	Pack (compress) the library.
RENAME	Rename a stream in the library.
REPLACE	Replace a stream in the library.
QUIT	End STRLIB without updating the library.

The following table describes characteristics of these commands:

Characteristic	Description
Case sensitivity	The Aspen Plus STRLIB program is not case sensitive. You can type your commands in either upper or lower case.
Partial matching of command	You can abbreviate commands. You only need to type enough letters to make the command unique. If the command you have typed is not unique, STRLIB displays a list of commands that begin with the letters you type. For example, if you type command **D**, and there is more than one command that starts with D, STRLIB lists all commands that start with D.
Incomplete commands	If you do not complete a command, or if a word cannot be recognized, STRLIB recognizes as much of the command as possible and displays a menu of possible command choices.
Canceling commands	At any subprompt away from the **STRLIB>** prompt, you can use the less than character (<) to cancel one item of the command. For example, if you enter **REPLACE**, the subprompt will appear as **STRLIB> REPLACE**. In order to get back to **STRLIB>** prompt, enter (<).
Initialization	You must initialize a new stream library before you can store any stream data

Description of STRLIB Commands

This section describes the commands you can use to create or modify a stream library.

ADD

Use this command to add a stream to the stream library. The ADD command copies a stream from the Aspen Plus summary file to the library. The stream to be copied must not already exist in the current case of the library. You can use the REPLACE command to replace streams that already exist.

You can specify ADD ALL to copy all streams from the summary file to the library.

```
STRLIB> ADD {sid}
            {ALL}
```

CASE

Use CASE to change the current case. Streams in the stream library are organized into cases. You establish a case when you open a summary file (using the OPEN command) or by using the CASE command. The ADD, DELSTREAM, DUMP, RENAME, and REPLACE commands apply to streams in the current case.

```
STRLIB> CASE casename
```

DELCASE

Use DELCASE to delete a case from the library. All streams in the case are also deleted.

```
STRLIB> DELCASE casename
```

DELSTREAM

Use DELSTREAM to delete a stream from the current case in the library. The stream must exist in the current case.

If you delete many streams from a library, you may wish to use the PACK command to recover the deleted space. See the PACK command description in this section.

```
STRLIB> DELSTREAM sid
```

DIRECTORY

Use DIRECTORY to list the cases and streams that are stored in the stream library. If you do not specify a case in the DIRECTORY command, STRLIB lists the cases in the library, and the number of streams in each case. If you specify a case, STRLIB lists the streams in that case.

```
STRLIB> DIRECTORY [casename]
```

DUMP

Use DUMP to write the information about a stream stored in the library to a file or to the terminal. STRLIB asks if you want to write to the terminal or to a file. If you want to write to a file, STRLIB prompts you for the file name. If you specify a stream ID, the stream must exist in the current case. You can specify DUMP ALL to dump all streams from a library. Aspen Plus dumps all streams from all cases.

The DUMP command is useful if you want to view the information for a stream, or if you want to transfer information from one library to another. If you need to reinitialize a library to increase the maximum number of cases that can be stored, use the DUMP ALL command first. This causes Aspen Plus to save the contents of the library. To restore the information, use the LOAD command.

```
STRLIB> DUMP {sid}
             {ALL}
```

END

Use this command to end the STRLIB session. Aspen Plus updates the stream library with the changes you make during the session. The END and EXIT commands are synonymous. (Use the QUIT command to end STRLIB without updating the library, so the changes made during the session are not saved.)

```
STRLIB> END
```

EXIT

Use EXIT to end the STRLIB session. Aspen Plus updates the stream library with the changes you make during the session. The END and EXIT commands are synonymous. (Use the QUIT command to end STRLIB without updating the library, so the changes made during the session are not saved.)

```
STRLIB> EXIT
```

HELP

Use HELP to invoke the interactive online help system, to obtain help for STRLIB commands.

```
STRLIB> HELP [command]
```

INITIALIZE

Use this command to initialize a new stream library. When you initialize a library, you must specify the maximum number of cases the library will contain. The INITIALIZE command must be entered before performing any operations on a new stream library.

The INITIALIZE command destroys all data in a stream library. It should only be used when creating a library, or after using the DUMP ALL command.

```
STRLIB> INITIALIZE numcase
```

LIST

Use this command to list the streams in the current summary file.

```
STRLIB> LIST
```

LOAD

Use this command to load information from a dump file created with the DUMP command. Aspen Plus loads all cases and streams.

```
STRLIB> LOAD filename
```

OPEN

Use this command to open a summary file, so that streams from an Aspen Plus run can be transferred to the library. You can specify an optional case name in the OPEN command. If you do not specify a case name, the RUNID from the summary file is used as the case name.

```
STRLIB> OPEN filename [casename]
```

PACK

Use this command to pack the stream library to recover blank spaces created when streams are deleted. The PACK command is necessary only if you delete many streams from a library and want to recover unused file space.

```
STRLIB> PACK
```

RENAME

Use this command to rename a stream in the library. The RENAME command applies only to the current case.

```
STRLIB> RENAME oldname newname
```

REPLACE

Use this command to replace a stream in the current case in the library, with a stream of the same name from the summary file. Aspen Plus adds the stream, if it does not exist in the library.

You can also specify REPLACE ALL to copy all streams from the summary file to the library, overwriting any streams of the same name that exist in the library.

STRLIB> REPLACE { **sid** / **ALL** }

QUIT

Use QUIT to end the STRLIB session. Aspen Plus does not update the stream library with any changes made during the current STRLIB session. Use the END or EXIT commands to end STRLIB and update the stream library with changes made during the session.

```
STRLIB> QUIT
```

Running STRLIB

You can run STRLIB both interactively and non-interactively, on all computers and operating systems.

Running STRLIB Interactively

Enter the STRLIB command to run the STRLIB program interactively at your operating system prompt:

STRLIB *libname*

Where *libname* is the name of the library you want to create or modify. It can be up to eight characters long.

The file name of the stream library for various operating systems is: libname.slb.

When the **STRLIB>** prompt appears, you must use the INITIALIZE command to initialize the maximum number of cases the library will contain. You are then ready to enter commands. Aspen Plus prompts you for each command. Online help is available for the commands. (See Description of STRLIB Commands, this chapter.)

Running STRLIB Non-interactively

You can run STRLIB non-interactively, to create or update a stream library. Running STRLIB non-interactively automatically adds all the streams from the

summary file produced by an Aspen Plus run to the library. The command to run STRLIB is:

```
strlib  libname  runid  [case]
```

Where:

libname	=	Name of the library you want to create or modify. If the librarydoes not exist, Aspen Plus creates and initializes it to contain10 cases.
runid	=	Name of the Aspen Plus summary file from which you wantto transfer streams
case	=	Case name in the library where you want to add streams.Specifying the case is optional. If you do not specify the casename, Aspen Plus uses the runid from the summary fileas the case name.

Retrieving Data from a Stream Library in Aspen Plus

Input Language for STREAM-LIB

```
STREAM-LIB
RETRIEVE  keyword=value
```

Keywords:

CASE STREAMS LIB-ID STATE SUBSTREAMS COMPS TRANSLATE

```
TRANSLATE  COMPS=(cid1  cid2)  (cid1  cid2) . . .
```

Input Language Description for STREAM-LIB

Use the STREAM-LIB paragraph in an Aspen Plus input file to specify the streams and information to be retrieved from an existing stream library. Stream libraries can store only material streams. You cannot retrieve information streams from a stream library.

If you have a STREAM paragraph for a stream, information in the STREAM paragraph is used instead of information retrieved from a stream library.

RETRIEVE

Use to specify the streams to retrieve. You must specify the case the streams belong to in the library (CASE) and the list of streams that will be filled in (STREAMS). You can also specify the components, substreams, and state variables to retrieve. You can have any number of RETRIEVE sentences. To retrieve data from a stream with a different stream ID, you must use LIB-ID to specify the ID of the stream in the library.

CASE	The case the streams belong to in the stream library. You can retrieve streams from more than one case by using more than one RETRIEVE sentence.
STREAMS	List of streams in the current simulation, that will be filled with data from the stream library. Use LIB-ID to specify the ID of the stream in the library, if the stream ID in the library does not match the stream ID in the current simulation. If you specify LIB-ID, you can specify only a single stream with the STREAMS keyword. You can specify STREAMS=ALL to retrieve all streams associated with the case in the library.

LIB-ID ..... ID of the stream in the stream library from which Aspen Plus retrieves data. Use LIB-ID only if you specify a single stream with the STREAMS keyword.

STATE ..... State variables to retrieve for the MIXED substream. Temperature, pressure, and vapor fraction are all stored in the stream library.

STATE = TP	Temperature and pressure (Default)
STATE = TV	Temperature and vapor fraction
STATE = PV	Pressure and vapor fraction

SUBSTREAMS ..... List of substreams to be retrieved from the stream library (Default=all substreams)

COMPS ..... List of components to be retrieved from the stream library (Default=all components)

TRANSLATE ..... List of component pairs to be mapped between the current simulation and the stream library. Each pair is enclosed in parentheses. The first element listed for each pair is the component ID in the current simulation. The second element is the component ID in the stream library. This mapping overrides the mapping specified in the translate sentence.

TRANSLATE

Use to specify component mapping between the current simulation and the stream library. The mapping is used for all streams retrieved, unless mapping is specified with the TRANSLATE keyword in the RETRIEVE sentence.

COMPS ..... List of component pairs that are to be mapped between the current simulation and the stream library. Each pair is enclosed in parentheses. The first element listed for each pair is the component ID in the current simulation. The second element is the component ID in the stream library.

Using a Stream Library in an Aspen Plus Run

You can specify which stream library Aspen Plus uses for a run. You can use only one stream library in an Aspen Plus run.

Aspen Plus uses the stream library pointed to by the environment variable USLB. You must set this environment variable in order for Aspen Plus to use it. The command to set the environment variable is:

```
SET USLB=libname
```

Where *libname* is the fully-qualified file name (disk name, directory name, and file name) for the stream library

44 Insert Libraries

This chapter describes the input language and commands for referencing insert libraries in an Aspen Plus simulation.

Inserts are Aspen Plus productivity tools that allow you to package a substantial amount of input for easy access. Many inserts are delivered with Aspen Plus. (See Chapter 8.) You can also write your own inserts.

To create and use an insert you must:

- Write the insert file. The insert file contains Aspen Plus input language for the insert.
- Reference the insert from an Aspen Plus input file.
- Build an insert library, using the MAKEINS procedure.
- Reference the insert library in an Aspen Plus run.

Writing Inserts

An insert consists of one or more Aspen Plus input language statements, followed by a line with the word END beginning in column one. Some inserts contain only static input language. Other inserts are more complex. They are true macros with variables that are filled in, based on arguments passed to the insert.

You can use your computer system text editor to create the insert file. Thee name of the insert file is *insname*.ins, where *insname* is the name of the insert. It must be a string of up to six characters. The string must follow the rules for Aspen Plus input language (see Chapter 1), and the rules for file names on your computer operating system.

This section discusses:

- Static inserts.
- Inserts with variable substitution.
- Rules for writing inserts.

Static Inserts

Static inserts contain the Aspen Plus input language paragraphs you normally use in an input file. The last line of the insert must be the word END, beginning in column one.

Static inserts can be used to define and package input language that you use in many Aspen Plus runs. For example, you can prepare an insert to:

- Define a standard units set. The insert contains the IN-UNITS and OUT-UNITS paragraphs for the units set that you commonly use.
- Define property parameters. The insert contains, for example, PROP-DATA paragraphs to define the data for a new component that does not appear in a data bank. The insert can be shared among users on a project to ensure consistency of results.
- Build property options. You can create an insert to build or modify a property option set. The insert contains the PROPERTIES, PROP-REPLACE, MP-ROUTE and SP-ROUTE paragraphs that specify the option set.
- Store assay information. The insert can contain the ASSAY, BLEND, and other paragraphs necessary to specify your assay for the Aspen Plus assay data analysis system. You can store a library of commonly-used feedstocks in an insert library.

Inserts with Variable Substitution

Although inserts containing static input language are useful for many applications, it is often desirable to pass parameters to an insert. Inserts in Aspen Plus can be used as true macros with argument substitution. You can write input language with dummy arguments that are replaced with actual arguments, when the insert is invoked in an input file.

When you write an insert with arguments, you use dummy arguments where you would normally use values or IDs (such as block IDs, component IDs, or stream IDs). Dummy arguments in an insert take the form %i, where % is a symbol indicating a dummy argument and i is the argument number. For example, the second dummy argument of an insert is expressed as %2.

Rules for Writing Inserts

Use the following rules when writing any type of insert:

- Insert names are limited to six characters.
- An insert can have any number of dummy arguments.
- A dummy argument can appear anywhere within an insert, even as part of a character string.
- If a dummy argument is to be concatenated with characters on its left, no special delimiter is required. For example, if TEMP=%1 is used in an insert, and the first actual argument to the insert is 300, the result is TEMP=300.
- If a dummy argument is to be concatenated with characters on its right, a special delimiter, the period (**.**), is required. The period is dropped when the dummy argument is replaced by an actual argument. For example, if SPEC=%3 is used in an insert, and the third actual argument is REAC, the result is REACSPEC.
- When a dummy argument is replaced by an actual argument, the line can be expanded beyond the usual 80-character limit. In this case, a continuation line is automatically generated. Continuation lines are not generated for inline FORTRAN statements.
- An insert can be any length, but must always end with an END statement that begins in column one.
- An insert can reference other inserts, as long as there is no recursion.

Referencing Inserts in Aspen Plus

Input Language for INSERT

```
INSERT   arg1   insname   arg2   arg3 ...
```

Input Language Description for INSERT

Use the INSERT paragraph to reference an insert in your input file.

INSERT

Use to invoke an insert. INSERT must begin in column one.

arg1 ..... Actual argument corresponding to the dummy argument %1. Use an asterisk (*) to skip *arg*1 if the referenced insert has no %1 dummy argument.

insname ..... Name of the insert. This is the same as the name of the insert file you create. The name of the insert can be no more than six characters long.

arg2, arg3, …… Actual arguments corresponding to the dummy arguments (such as %2 and %3)

Building an Insert Library with MAKEINS

After you create your insert files, you must build an insert library. Aspen Plus can only retrieve inserts from an insert library. To create an insert library execute the following command: **makeins**. Aspen Plus creates a library called USER. The file name of the insert library is user.ilb.

Using an Insert Library in an Aspen Plus Run

You can specify which insert library Aspen Plus will use for a run. The insert library used is determined by the following rules:

- You can specify the name of an insert library in the environment variable UILB.
- If you do not specify a library in the environment variable UILB, Aspen Plus will search for an insert library named *user* in your directory. If this library exists, it is used for the Aspen Plus run.

You can set the UILB environment variable so that Aspen Plus can use it. The command to set UILB is:

```
SET UILB=libname
```

Where *libname* is the fully-qualified file name (disk name, directory name, and file name) for the insert library.

45 Simulation Options, Limits, and Diagnostics

This chapter describes the input language for specifying simulation options, limits, diagnostics levels, and system options.

Use this paragraph	To specify
SIM-OPTIONS	Simulation options and global limits for temperature and pressure
RUN-CONTROL	Run time and error limits
DIAGNOSTICS	Diagnostic levels and print limits
SYS-OPTIONS	System options that affect error checking and inline FORTRAN errors
ACCOUNT-INFO	Information for the Aspen Plus run accounting report
DISABLE	Deactivate streams, blocks, and other flowsheet objects

Simulation Options

Input Language for SIM-OPTIONS

SIM-OPTIONS	*keyword=value*

Optional keywords:

ENERGY-BAL RESTART FREE-WATER TLOWER TUPPER PLOWER PUPPER FLASH-MAXIT FLASH-TOL MW-CALC ROOT-EXTR ATM-PRES BYPASS-PROP STOIC-MB-CHECK STOIC-MB-TOL MASS-BAL-CHECK NPHASE PHASE PROP-DERIV PARADIGM MAXSOL-CHECK DX-REQUIRED DN-REQUIRED BRE-FLASH SOLID-DERIV XW-H2OPHASE

Input Language Description for SIM-OPTIONS

ENERGY-BAL	**ENERGY-BAL=NO**	Performs only mass balance calculations
	ENERGY-BAL=YES	Performs energy and mass balance calculations (Default)
RESTART	**RESTART=NO**	Initializes calculations at each pass
	RESTART=YES	Uses results from previous convergence pass as initial estimate for next pass (Default)
FREE-WATER	**FREE-WATER=NO**	Does not perform free-water calculations (Default)
	FREE-WATER=YES	Performs free-water calculations
TLOWER	Lower limit on temperature (Default=10 K)	
TUPPER	Upper limit on temperature (Default=10000 K)	
PLOWER	Lower limit on pressure (Default=0)	
PUPPER	Upper limit on pressure (Default=$1x10^{10}$ N/m^2)	
FLASH-MAXIT	Maximum number of iterations for flash calculations (Default=30)	
FLASH-TOL	Tolerance for flash calculations (Default=$1x10^{-4}$)	
MW-CALC	**MW-CALC=NO**	Does not calculate molecular weight
	MW-CALC=YES	Calculates molecular weight from atomic number and weight (Default)
ROOT-EXTR	Threshold on volume slope of isotherms, below which equation-of-state is extrapolated (Default=0.1)	
ATM-PRES	Ambient or atmospheric pressure for gauge pressure calculations (Default=101325 N/m^2)	
BYPASS-PROP	**BYPASS-PROP=NO**	Performs PROP-SET calculations, even if flash errors occur
	BYPASS-PROP=YES	Does not perform PROP-SET calculations if flash errors occur (Default)
STOIC-MB-CHECK	**STOIC-MB-CHECK= WARNING**	Gives warning messages during input checking if reaction stoichiometry violates mass balance
	STOIC-MB-CHECK= ERROR	Gives error messages during input checking if reaction stoichiometry violates mass balance (Default)

STOIC-MB-TOL	Tolerance used in checking reaction stoichiometry for mass balance (Default=1)	
MASS-BAL-CHECK	**MASS-BAL-CHECK=YES**	Performs mass balance check around each block as it is executed, and again after simulation is complete (Default)
	MASS-BAL-CHECK=NO	Does not perform mass balance checking
NPHASE	Maximum number of phases in MIXED substream. Use to override the default for NPHASE in UOS blocks and input paragraphs. (See Table 46.1.)	
	NPHASE=1	One-phase calculation
	NPHASE=2	Two-phase calculation
	NPHASE=3	Three-phase calculation
PHASE	Specifies the phase when NPHASE=1. Use to override the default for PHASE in UOS blocks and input paragraphs. (See Table 46.1.)	
	PHASE=V	Vapor (Default)
	PHASE=L	Liquid
PROP-DERIV	Specifies the use of analytical derivatives (default) versus finite difference numerical approximation of the property derivatives.	
	PROP-DERIV= ANALYTICAL	Use analytical derivatives (Default)
	PROP-DERIV= NUMERICAL	Use numerical estimates
PARADIGM	Specifies the flowsheet solution mode.	
	PARADIGM=SM	Use the traditional block-by-block sequential modular approach to solve the flowsheet (Default)
	PARADIGM=EO	Use the new equation-oriented approach to solve the whole flowsheet simultaneously after initializing the flowsheet with sequential modular approach. See Chapter 48 for Equation-Oriented Solution.
	PARADIGM=MIXED	This is a hybrid of the two options above. In the MIXED mode, you can solve hierarchies with equation-oriented approach but solve the whole flowsheet with sequential modular approach. You specify the solution method of a hierarchy and its subhierarchies with the SOLVE paragraph in Chapter 48. Note that the solution method of the SOLVE paragraph is only used when PARADIGM=MIXED is enabled. Also note that EO hierarchies are always solved in the simulation mode.
MAXSOL-CHECK	**MAXSOL-CHECK=YES**	Limit water solubility in the hydrocarbon phase. This option prevents water solubility from becoming unreasonably large due to extrapolation beyond its range of validity (usually about 50ºC). (Default)
	MAXSOL-CHECK=NO	Do not limit water solubility in the hydrocarbon phase.
DX-REQUIRED	**DX-REQUIRED=NO**	Do not require calculations of molar fraction derivatives (d/dx_i) in the simulation. This option can save significant memory. (Default)
	DX-REQUIRED=YES	Require calculations of molar fraction derivatives (d/dx_i). These derivatives are not currently used by any Aspen Plus equation-oriented model, but may be used by some imported models from Aspen Custom Modeler.

DN-REQUIRED	**DN-REQUIRED=YES**	Require calculations of molar flow derivatives (d/dn_i) in the simulation. Molar flow derivatives are used in equation-based simulation and required by most unit operation models. (Default)
	DN-REQUIRED=NO	Do not require calculations of molar flow derivatives (d/dn_i). This option can save significant memory.
BRE-FLASH.....	**BRE-FLASH=YES**	Use flash algorithm of Bryan Research & Engineering when BRE property methods are used. (Default) **Note:** BRE property methods require a separate license for BRE. This option has no effect when other property methods are used.
	BRE-FLASH=NO	Do not use flash algorithm of BR&E.
SOLID-DERIV.....	**SOLID-DERIV=NO**	Do not require derivatives of solid properties (d/dx_i and d/dn_i) in the simulation. This option can save significant memory. (Default)
	SOLID-DERIV=YES	Require derivatives for solid properties (d/dx_i and d/dn_i). Solid property derivatives are used in equation-based simulation involving conventional solids, including electrolyte salts.

XW-H2OPHASE ..... Minimum value of water mole fraction in the water-rich phase, above which the hydrocarbon solubility model (dirty-water method) is applied. (Default = 0.98).

Table 46.1 Overriding Defaults for NPHASE and PHASE

UOS Model/Input Paragraph	Sentences	Keywords
STREAM	—	NPHASE, PHASE
MIXER	PARAM	NPHASE, PHASE
FSPLIT	PARAM	NPHASE, PHASE
SSPLIT	PARAM	NPHASE, PHASE
SEP	PARAM	NPHASE, PHASE
	FLASH-SPECS	NPHASE, PHASE
SEP2	PARAM	NPHASE, PHASE
	FLASH-SPECS	NPHASE, PHASE
HEATER	PARAM	NPHASE, PHASE
FLASH2	PARAM	NPHASE†
HEATX	FLASH-SPECS	NPHASE, PHASE
MHEATX	HOT-SIDE	NPHASE, PHASE
	COLD-SIDE	NPHASE, PHASE
RSTOIC	PARAM	NPHASE, PHASE
RYIELD	PARAM	NPHASE, PHASE
REQUIL	PARAM	NPHASE, PHASE††
RGIBBS	PARAM	NPHASE, VAPOR†††
RCSTR	PARAM	NPHASE, PHASE
RPLUG	PARAM	NPHASE, PHASE
	COOLANT	NPHASE, PHASE
COOLANT	PARAM	NPHASE, PHASE
RBATCH	PARAM	NPHASE, PHASE, NPHASE-ACCUM, PHASE-ACCUM
PUMP	PARAM	NPHASE
COMPR	PARAM	NPHASE
MCOMPR	PARAM	COMPR-NPHASE, COOLER-NPHASE
PIPELINE	PARAM	NPHASE, PHASE
PIPE	PARAM	NPHASE, PHASE
VALVE	PARAM	NPHASE, PHASE
CRYSTALLIZER	PARAM	NPHASE
USER	FLASH-SPECS	NPHASE, PHASE
USER2	FLASH-SPECS	NPHASE, PHASE
CALCULATOR	FLASH-SPECS	NPHASE, PHASE
TRANSFER	FLASH-SPECS	NPHASE, PHASE
BALANCE	FLASH-SPECS	NPHASE, PHASE
PROP-TABLE		
FLASHCURVE	PARAM	NPHASE†
RESIDUE	PARAM	NPHASE†
PRES-RELIEF	PARAM	NPHASE, VENT-NPHASE, VENT-PHASE

† If NPHASE is set to 1 in SIM-OPTIONS, the local NPHASE is set to 2.

†† If NPHASE is set to 3 in SIM-OPTIONS, the local NPHASE is set to 2.

††† In SIM-OPTIONS, if NPHASE is set to 1 and PHASE is set to L, the local VAPOR is set to NO.

Time and Error Limits

Input Language for RUN-CONTROL

RUN-CONTROL *keyword=value*

Optional keywords:

MAX-TIME MAX-ERRORS

Input Language Description for RUN-CONTROL

MAX-TIME ..... Simulation time limit in seconds. This limit applies only to the actual simulation execution and excludes the input translation. (Default=120)

MAX-ERRORS ..... Error limit for all level 1 and 2 errors. (See Table 46.2.) (Default=50)

Table 46.2 Message Levels

Level	Message	Description
0	Terminal error	Only terminal error messages are listed. Execution cannot continue.
1	Severe error	Level 0 and severe error messages are listed. Execution can continue, but subsequent processing is likely to be erroneous.
2	Error	Level 1 and error messages are listed. Execution can continue, but subsequent processing is likely to be erroneous.
3	Warning	Level 2 and warnings are listed. Execution can continue, but a condition has been encountered that you should be aware of. (For example, a correlation has been extrapolated beyond its normal limits.)
4	Information	Level 3 and brief diagnostic information are listed. Messages allow you to trace the progress of a run.
5-8	Diagnostic	Level 4 and additional diagnostics and information on flowsheet sequencing are listed. Messages can be used to analyze convergence and simulation problems. The amount of information listed increases with each level.

Diagnostic Levels and Print Limits

Input Language for DIAGNOSTICS

DIAGNOSTICS
HISTORY *keyword=value*

Keywords:

SYS-LEVEL SIM-LEVEL PROP-LEVEL STREAM-LEVEL CONV-LEVEL VAR-LEVEL INSERT SORTED

TERMINAL *keyword=value*

Keywords:

SIM-LEVEL CONV-LEVEL VAR-LEVEL

MAX-PRINT *keyword=value*

Optional keywords:

SYS-LIMIT SIM-LIMIT PROP-LIMIT

Input Language Description for DIAGNOSTICS

HISTORY

Use to enter diagnostic message levels printed in the history file, and to control printing of the insert file echo and sorted input echo. The level is defined from 0 to 10. The amount of information listed increases with each level. (See Table 46.2.)

SYS-LEVEL	Sets level of input translator errors and diagnostics printed in history file (Default=4)	
SIM-LEVEL	Sets level of simulation errors and diagnostics printed in history file (Default=4)	
PROP-LEVEL.....	Sets level of physical property errors and diagnostics printed in history file (Default=4)	
STREAM-LEVEL.....	Sets level of stream diagnostics printed in history file (Default=4)	
CONV-LEVEL	Sets level of convergence diagnostics printed in history file (Default=4)	
VAR-LEVEL.....	Sets the level of diagnostics printed in the history file for FORTRAN variables used in the DEFINE and VECTOR-DEF sentences of CALCULATOR, DESIGN-SPEC, SENSITIVITY, OPTIMIZATION, and CONSTRAINT blocks. Diagnostic levels are:	
	VAR-LEVEL=0,1,2,3,4	No diagnostics
	VAR-LEVEL=5	Prints values of accessed FORTRAN variables written back to flowsheet variables (WRITE-VARS)
	VAR-LEVEL=6	Prints VAR-LEVEL=5 diagnostics and initial values of all accessed FORTRAN variables (READ-VARS and WRITE-VARS)
INSERT	**INSERT=YES**	Echoes insert files in the history file (Default)
	INSERT=NO	Suppresses insert echo
SORTED	**SORTED=YES**	Prints sorted input file (including inserts) in the history file only when inserts are present (Default)
	SORTED=NO	Does not print sorted input file

TERMINAL

Use to enter diagnostic message levels printed in the log file or to the terminal. The level is defined from 0 to 10. The amount of information listed increases with each level (see Table 46.2).

SIM-LEVEL	Sets level of simulation errors and diagnostics printed in the log file or to the terminal (Default=4)
CONV-LEVEL	Sets level of convergence diagnostics printed in log file or to the terminal (Default=4)

VAR-LEVEL	Sets the level of diagnostics printed in the log file or to the terminal for FORTRAN variables used in the DEFINE and VECTOR-DEF sentences of CALCULATOR, DESIGN-SPEC, SENSITIVITY, OPTIMIZATION, and CONSTRAINT blocks. Diagnostic levels are:	
	VAR-LEVEL=0,1,2,3,4	No diagnostics
	VAR-LEVEL=5	Prints values of accessed FORTRAN variables written back to flowsheet variables (WRITE-VARS)
	VAR-LEVEL=6	Prints VAR-LEVEL=5 diagnostics and initial values of all accessed FORTRAN variables (READ-VARS and WRITE-VARS)

MAX-PRINT Use to set print limits for errors and warnings.

SYS-LIMIT	Maximum number of input translator errors and warnings printed in the history file (Default=200)
SIM-LIMIT	Maximum number of simulation and convergence errors and warnings printed in the history file (Default=200)
PROP-LIMIT	Maximum number of physical property errors and warnings printed in the history file (Default=200)

System Options

Input Language for SYS-OPTIONS

SYS-OPTIONS *keyword=value*

Optional keywords:

INTERPRET TRACE BLOCK-CHECK

Input Language Description for SYS-OPTIONS

INTERPRET	Controls whether inline FORTRAN statements are interpreted at execution time, or are compiled into the generated FORTRAN program	
	INTERPRET=YES	Interprets FORTRAN statements whenever possible (Default)
	INTERPRET=NO	Compiles all FORTRAN statements
TRACE	Controls whether FORTRAN tracebacks will be printed in the history file, when a FORTRAN error or an Aspen Plus terminal error occurs	
	TRACE=YES	Prints tracebacks
	TRACE=NO	Suppresses tracebacks (Default)
BLOCK-CHECK	**BLOCK-CHECK=YES**	Checks unit operation block input for specification errors and inconsistencies (Default)
	BLOCK-CHECK=NO	Does not check block input

Accounting Information

Input Language for ACCOUNT-INFO

```
ACCOUNT-INFO    keyword=value
```

Optional keywords:

ACCOUNT PROJECT-ID PROJECT-NAME USER-NAME

Input Language Description for ACCOUNT-INFO

ACCOUNT ..... Account number (up to eight digits)

PROJECT-ID ..... Project ID (up to eight characters)

PROJECT-NAME ..... String of up to 32 characters enclosed in quotes (")

USER-NAME ..... String of up to 20 characters enclosed in quotes (")

Deactivating Simulation Objects

Input Language for DISABLE

```
DISABLE
object-type    id
```

Object types supported:

BLOCK STREAM CONNECTION CONVERGENCE COST-BLOCK
SENSITIVITY TRANSFER FORTRAN UTILITY ECONOMICS
CASE-STUDY BALANCE PRES-RELIEF REGRESSION SEQUENCE
DESIGN-SPEC CONSTRAINT OPTIMIZATION PPTABLE PROP-TABLE

Input Language Description for DISABLE

unit-type ..... Specifies the type of simulation object to be deactivated. Note that deactivating an object may cause other objects to be deactivated by association. See the *Aspen Plus User Guide* for more information on deactivating blocks.

id ..... Specifies the id of the object to be deactivated.

46 Report Options

This chapter describes the input language for specifying report options. This chapter discusses:

- How to tailor the report file.
- Batch stream report.
- Report scaling.
- Print-plots.

Tailoring the Report File

Input Language

```
TITLE   "a title description - up to 64 characters enclosed in quotes"
DESCRIPTION   "any amount of text, entered on any number of lines, and enclosed
in quotes"
REPORT   reportopt-list   [LINES=value]   [WIDE=value]
```

Reportopts:

NOREPORT INPUT NOINSERT NOADA NOFLOWSHEET NOSENSITIVITY NOPROPERTIES NOBLOCKS NOSTREAMS

```
ADA-REPORT   ada-reportopt-list
```

ADA-reportopts:

NOCURVES NOCOMPS PARAMS

```
FLOWSHEET-REPORT   flow-reportopt-list
```

Flow-reportopts:

NODESCRIPTION NOTOTBAL NOCOMPBAL NOFORTRAN NODESIGN-SPEC NOCONSTRAINT NOOPTIMIZATION NOTRANSFER NOCONVERGENCE NOSEQUENCE

```
PROPERTY-REPORT   prop-reportopt-list
```

Prop-reportopts:

NOCOMPS PARAMS PCES PROP-DATA NOPCES NOPROP-DATA DFMS PROJECT

```
BLOCK-REPORT   block-reportopt-list   INCL-BLOCKS=blockid-list   &
 EXCL-BLOCKS=blockid-list
```

Block-reportopts:

NEWPAGE NOSORT NOTOTBAL NOINPUT COMPBAL NORESULTS NOREPORT

```
STREAM-REPORT   stream-reportopt-list   PROPERTIES=propsetid-list  &
       INCL-STREAMS=sid-list   EXCL-STREAMS=sid-list
SUPPLEMENTARY   supno   stream-reportopt-list   PROPERTIES=propsetid-list  &
       INCL-STREAMS=sid-list   EXCL-STREAMS=sid-list   keyword=value
```

Stream-reportopts:

NOREPORT WIDE NOSORT NOZEROFLOW NOMOLEFLOW MASSFLOW STDVOLFLOW MOLEFRAC MASSFRAC STDVOLFRAC STRUCTURE NOATTR-DESC NOCOMP-ATTR NOSUBS-ATTR

Optional keywords:

PRINT-PLOT HEADING WIDE GRID INTERPOLATE SUBROUTINE

Input Language Description for REPORT

reportopt-list ..... List of global report options:

NOREPORT	Suppresses entire report
INPUT	Specifies that the input file is printed
NOINSERT	Suppresses insert file echo when the input file is printed
NOADA	Suppresses the assay data analysis report
NOFLOWSHEET	Suppresses flowsheet report
NOSENSITIVITY	Suppresses sensitivity report
NOPROPERTIES	Suppresses property report
NOBLOCKS	Suppresses unit operation block report
NOSTREAMS	Suppresses stream report

(Default is to report all sections except the input file)

LINES..... Number of lines to be printed per page in the report (Default=60)

WIDE ..... Plot option. This option overrides the default established by the PLOT-OPTIONS paragraph. (See Print Plots, this chapter.)

Input Language Description for ADA-REPORT

ada-reportopt-list ..... List of report options for ADA report:

NOCURVES	Suppresses the distillation curve report
NOCOMPS	Suppresses the listing of generated pseudocomponents
PARAMS	Specifies that the values (in SI units) of all pseudocomponent property parameters are to be reported

(Default is to report all sections except the pseudocomponent property parameter section)

Input Language Description for FLOWSHEET-REPORT

flow-reportopt-list ..... List of report options for flowsheet reports:

NODESCRIPTION	Suppresses descriptions of flowsheet connectivity, report scaling, design specifications, constraints, and optimization problems. This option also suppresses description for Calculator, transfer, case-study, and sensitivity blocks
NOTOTBAL	Suppresses total mass and energy balances around the flowsheet
NOCOMPBAL	Suppresses component mass balances around the flowsheet
NOFORTRAN	Suppresses Calculator block report
NODESIGN-SPEC	Suppresses design-spec report
NOCONSTRAINT	Suppresses constraint report
NOOPTIMIZATION	Suppresses optimization problem report
NOTRANSFER	Suppresses transfer block report
NOCONVERGENCE	Suppresses convergence block report
NOSEQUENCE	Suppresses calculation sequence report

(Default is to report all sections)

Input Language Description for PROPERTY-REPORT

prop-reportopt-list..... List of report options for property report. Use PCES and PROP-DATA only when the property constant estimation system is used in simulation or in table generation system (TGS) runs. In simulation or TGS runs, the default is to suppress the property parameter report and the project data file reports. Use NOPCES and NOPROP-DATA in stand-alone PCES runs only. In stand-alone PCES runs, the default is to generate the property parameter report and the project data file.

NOCOMPS	Suppresses the listing of component IDs, formulas, names, and aliases used in the simulation
PARAMS	Specifies that the values (in SI units) of all of physical property parameters used in the simulation are to be reported
PCES	Specifies that property constant estimation results are to be reported
PROP-DATA	Specifies that a PROP-DATA paragraph containing the results of property constant estimation is to be generated
NOPCES	Suppresses the property constant estimation report
NOPROP-DATA	Suppresses the generation of the PROP-DATA paragraph
DFMS	Specifies that the data file management system input file is generated
PROJECT	Specifies that the project data file is to be generated

(Default is to report the list of components and suppress the property parameter report and project data file)

Input Language Description for BLOCK-REPORT

block-reportopt-list .... List of report options for block reports:

NEWPAGE	Specifies that each block report is to begin on a new page
NOSORT	Suppresses alphabetic block sort
NOTOTBAL	Suppresses total mass and energy balances around the block
NOINPUT	Suppresses the summary of user input and system defaults
COMPBAL	Specifies that the component mass balances around the block are to be reported
NORESULTS	Suppresses block results
NOREPORT	Suppresses the entire block report

(The BLOCK-REPORT paragraph is hierarchical. The default at the top level is to report all sections except the component mass balance and to use the new page option. The default for hierarchy blocks is the list of the above block report options specified for the parent hierarchy.)

INCL-BLOCKS..... List of unit operation blocks to be included in the report. Blocks are printed in the order listed. You cannot use both INCL-BLOCKS and EXCL-BLOCKS. (If you do not use either option, Aspen Plus reports all blocks.)

EXCL-BLOCKS..... List of unit operation blocks to be excluded from the report

Input Language Description for STREAM-REPORT

stream-reportopt-list.. List of report options for stream report:

NOREPORT	Suppresses the standard stream report. Supplementary reports can still be generated.
WIDE	Prints ten streams, instead of five, across the page. (132 columns are used.)
NOSORT	Suppresses alphabetic stream sort
NOZEROFLOW	Suppresses printing of components with zero flow or fraction
MOLEFLOW, MASSFLOW, STDVOLFLOW, MOLEFRAC, MASSFRAC, STDVOLFRAC	Specifies whether to report component flows or fractions on a mole, mass, or standard- liquid-volume basis. You can use as many of these options as desired in any stream report. (Default=MOLEFLOW)
STRUCTURE	Specifies printing stream structure information
NOATTR-DESC	Suppresses particle size distribution size limits
NOCOMP-ATTR	Suppresses component attribute values
NOSUBS-ATTR	Suppresses substream attribute values

(The STREAM-REPORT paragraph is hierarchical. The default for hierarchy blocks is the list of stream report options besides INCL-STREAMS and EXCL-STREAMS specified for the parent hierarchy.)

PROPERTIES ..... List of property set IDs. (See Chapter 41.)

INCL-STREAMS ..... List of streams to be included in the report. Streams are printed in the order listed. You cannot use both INCL-STREAMS and EXCL-STREAMS. (If you do not use either option, Aspen Plus prints all streams.)

EXCL-STREAMS ..... List of streams to be excluded from the report

SUPPLEMENTARY Use to generate supplementary stream reports.

supno..... Supplementary report number

stream-reportopt-list.. The same report options listed in the STREAM-REPORT section, for *stream-reportopt-list*

PROPERTIES ..... List of property set IDs for the properties to be printed. (See Chapter 41.)

INCL-STREAMS ..... List of streams to be included in the report. Streams are printed in the order listed. You cannot use both INCL-STREAMS and EXCL-STREAMS. (If you do not use either option, Aspen Plus prints all streams.)

EXCL-STREAMS ..... List of streams to be excluded from the report

PRINT-PLOT..... Plots can be generated only when the properties TBPCRV, D86CRV, D1160CRV and/or VACCRV are included in a PROP-SET listed in the PROPERTIES *propsetid-list* for the supplementary stream report.

PRINT-PLOT=YES	Generates print-plots of distillation temperature versus the percent distilled (Default)
PRINT-PLOT=NO	Does not generate print-plots

HEADING ..... Heading of up to 64 characters enclosed in quotes. The heading is printed at the top of the print-plot, and passed to the user stream report subroutine.

WIDE, GRID, INTERPOLATE ..... Plot options. Use to override defaults established by the PLOT-OPTIONS paragraph. (See Print Plots, this chapter.)

SUBROUTINE ..... User-supplied stream report subroutine name. For details on writing user-supplied stream report subroutine, see *Aspen Plus User Models*, Chapter 8.

Batch Stream Report

Input Language for BATCH-OPERATION

```
BATCH-OPERATION
STREAMS    sid    cycle-time    down-time    op-time    ntrain  / ...
```

Input Language Description for BATCH-OPERATION

STREAMS

Use to designate batch streams, and specify the number of parallel trains for these streams. You can also enter the following batch times: cycle, operation, and down. You can specify just cycle time, or any two of the three times.

sid..... Stream ID

cycle-time..... Total time of batch cycle

down-time..... Down time during total batch cycle (Default=0)

op-time..... Operation time during total batch cycle. An operation time of zero indicates an instantaneous batch charge or discharge. *op-time* cannot be greater than *cycle-time*.

ntrain..... Number of parallel trains for batch operation

Report Scaling

The reports produced by an Aspen Plus simulation can be scaled, using the REPORT-SCALE paragraph. You can scale a report so that a designated simulation result obtains a required value. The designated simulation result can be any flowsheet variable accessed directly using a DEFINE or VECTOR-DEF sentence. (See Chapter 29.) Or the designated result can be a function of accessed flowsheet variables computed using inline FORTRAN statements. (See Chapter 31 and the *Aspen Plus User Guide*.) The designated result must be affected by scaling. (For example, a flow is acceptable; a fraction or ratio is not acceptable.)

Report scaling affects only the values printed in the report. It has no effect on simulation computations. Sensitivity tables are not scaled. (See Chapter 35.)

There can be only one REPORT-SCALE paragraph in an Aspen Plus input file. It applies to the base case and all case studies, but has no effect on sensitivity reports.

Accessed flowsheet variables, with the exception of VECTOR-DEF, are in the units established by the IN-UNITS statement. Unit options in brackets or braces cannot be used.

Input Language for REPORT-SCALE

```
REPORT-SCALE
F          FORTRAN Declaration Statements
DEFINE   fvar   vartype   keyword=value
VECTOR-DEF   farray   vectype   sid
F          Executable FORTRAN Statements
SCALE   "expression1"   TO   "expression2"
```

Input Language Description for REPORT-SCALE

DEFINE, VECTOR-DEF

Use to access a flowsheet variable and equivalence it to the FORTRAN variable *fvar*. Use *fvar* in subsequent FORTRAN statements or SCALE expressions to represent the flowsheet variable. VECTOR-DEF is similar to DEFINE, except that VECTOR-DEF equivalences an entire stream or block profile result to the FORTRAN array, *farray*. At least one DEFINE or VECTOR-DEF sentence must appear in a REPORT-SCALE paragraph. See Chapters 29 and 30 for a complete description of the DEFINE and VECTOR-DEF sentences.

FORTRAN Statements

Any valid FORTRAN statement subject to the restrictions discussed in the *Aspen Plus User Guide* and Chapter 31. FORTRAN comments (not shown) can also be used. FORTRAN statements are needed only if the desired scaling is too complex to be represented using SCALE expressions.

SCALE

Use to establish desired report scaling. The scale factor is:

expression2 / expression1

Where expression1 and expression2 are any valid FORTRAN arithmetic expressions

Typically, expression1 is a single FORTRAN variable and expression2 is the desired value for the variable. In this case the quotes (") can be omitted. The scale factor is computed after all simulation calculations are complete. It is applied to all extensive variables in the report, except to those in the flowsheet section of the report.

Print-Plots

Input Language for PLOT-OPTIONS

```
PLOT-OPTIONS    keyword=value
```

Optional keywords:

WIDE GRID INTERPOLATE

Input Language Description for PLOT-OPTIONS

WIDE	**WIDE=YES**	132 character width plot
	WIDE=NO	80 character width plot (Default)
GRID	**GRID=YES**	Prints the grid on the plot (Default)
	GRID=NO	Does not print the grid
INTERPOLATE	**INTERPOLATE=YES**	Prints interpolation characters between plot points (Default)
	INTERPOLATE=NO	Does not print interpolation characters

47 Modifying and Restarting Simulations

This chapter describes the input language for creating an edit run input file. The Aspen Plus edit run capability lets you retrieve the Problem Definition File (APPDF) from a previous run, modify or add to the problem, and restart the calculations.

This chapter also includes instructions on how to run an edit file. It describes how to restart simulation calculations for a problem that has not yet converged. In this case many input processing steps are bypassed, and the simulation calculations begin with the retrieved stream and block results. The edit run capability saves computer time, and makes it easy to reconverge recycle problems when you make modifications or perform case studies.

Creating an Edit Run Input File

You must create a new input file for an edit run. This file has EDIT as the first line. It contains only those paragraphs that change the problem specifications or run options from the previous run. Table 48.1 lists the paragraphs that can be used in an edit run. Any paragraph not listed is automatically skipped by Aspen Plus and has no effect on the run.

In most cases the paragraphs used in an edit run completely replace the corresponding specifications from the previous run. You must enter the complete paragraph, just as in a standard Aspen Plus run. In a few cases, as indicated in Table 48.1, the replacement occurs at the sentence or individual entry level. In these few cases you need to enter only the specifications that change.

Table 47.1 Paragraphs Used in Edit Runs

Paragraph	Replacement Level
ADVENT	Paragraph
BALANCE	Paragraph
BLOCK	Paragraph
BLOCK-REPORT	Paragraph†
CALCULATOR	Paragraph
CASE-STUDY	Paragraph
COMP-GROUP	Paragraph
CONSTRAINT	Paragraph (Note 1)
CONV-OPTIONS	Paragraph
CONV-ORDER	Paragraph
CONVERGENCE	Paragraph
DATA-SET	Paragraph
DEF-STREAMS	††
DEF-STREAM-ATTR	††
DEF-STREAM-CLASS	††
DEF-SUBS	††
DEF-SUBS-ATTR	††
DEF-SUBS-CLASS	††
DELETE	Paragraph
DESCRIPTION	Paragraph
DESIGN-SPEC	Paragraph (Note 2)
DIAGNOSTICS	Paragraph
FLOWSHEET	Sentence
FLOWSHEET-REPORT	Paragraph

† BLOCK-REPORT options cannot be changed in an edit run. However, INCL-BLOCKS or EXCL-BLOCKS lists can be replaced.

†† These paragraphs cannot be used to change the stream or substream class and attributes of any streams or flowsheet sections from the previous run. They can be used in an edit run to define the stream or substream class of new streams or flowsheet sections.

continued

Table 47.1 Paragraphs Used in Edit Runs (continued)

Paragraph	Replacement Level
IN-UNITS	Paragraph†††
OPTIMIZATION	Paragraph (Note 2)
OUT-UNITS	Paragraph
PRES-RELIEF	Paragraph
PROFILE-DATA	Paragraph
PROP-SET	Paragraph♦
PROP-TABLE	Paragraph
PROPERTY-REPORT	Paragraph
REACTIONS	Paragraph
REGRESSION	Paragraph
REPORT	Paragraph
REPORT-SCALE	Paragraph
RUN-CONTROL	Individual Entry
SENSITIVITY	Paragraph
SEQUENCE	Paragraph
SIM-OPTIONS	Individual Entry
SIMULATE/NOSIMULATE	Individual Entry
STREAM	Paragraph
STREAM-LIBRARY	Paragraph
STREAM-REPORT	Paragraph
SUMMARY/NOSUMMARY	Paragraph
SYS-OPTIONS	Individual Entry
TEAR	Paragraph
TITLE	Paragraph
TRANSFER	Paragraph
USER-PROPERTY	Paragraph

† BLOCK-REPORT options cannot be changed in an edit run. However, INCL-BLOCKS or EXCL-BLOCKS lists can be replaced.

†† These paragraphs cannot be used to change the stream or substream class and attributes of any streams or flowsheet sections from the previous run. They can be used in an edit run to define the stream or substream class of new streams or flowsheet sections.

††† In an edit run the IN-UNITS paragraph affects only those values entered in the edit run. Values entered in previous run(s) are not changed.

♦ You cannot use the PROP-SET paragraph to change entries for an ID defined in a previous run. You can use the PROP-SET paragraph to define new IDs used in an edit run.

FLOWSHEET Paragraph

The FLOWSHEET paragraph is used differently in edit runs. SIM-OPTIONS has additional entries that are used only in edit runs. Three special paragraphs, DELETE, SIMULATE, and NOSIMULATE, can be used in edit runs.

Input Language for FLOWSHEET

```
FLOWSHEET    [sectionid]
BLOCK    blockid    IN=sid-list    OUT=sid-list
```

Input Language Description for FLOWSHEET

Use the FLOWSHEET paragraph in an edit run to change the flowsheet connectivity. Use the BLOCK sentence to add a new unit operation block to the flowsheet, or to change the inlet and outlet streams of an existing block. You do not need to enter blocks where inlet and outlet streams are not changed. You can introduce new streams into the flowsheet by entering them in a BLOCK sentence.

When the flowsheet is divided into sections, you must enter a FLOWSHEET paragraph for each added or modified section.

sectionid	Flowsheet section ID (required when the flowsheet from the previous run contained more than one section)
blockid	Unit operation block ID. Can be hierarchical; see Chapter 9 for naming conventions and restrictions.
sid-list	List of stream IDs

SIM-OPTIONS Paragraph

Input Language for SIM-OPTIONS

SIM-OPTIONS	*keyword=value*

Optional keywords:

ENERGY-BAL FREE-WATER RESTART REINIT-BLOCKS REINIT-STREAMS TLOWER TUPPER PLOWER PUPPER BYPASS-PROP STOIC-MB-CHECK STOIC-MB-TOL MASS-BAL-CHECK ATM-PRES FLASH-MAXIT FLASH-TOL NPHASE PHASE PARADIGM

Input Language Description for SIM-OPTIONS

Use the SIM-OPTIONS paragraph in an edit run to reset convergence block and unit operation block restart flags; to restore tear streams or streams manipulated by design specifications or by Calculator blocks to their original values; and to reset any other flowsheet stream to zero flow. It is usually most efficient to begin calculations with the block and stream results from the previous run. You can also use SIM-OPTIONS to request mass-balance-only simulation, to change free-water simulation options, to reduce the flash tolerance, or to increase the maximum number of flash iterations. (See Chapter 45.)

ENERGY-BAL	**ENERGY-BAL=NO**	Performs only mass balance calculations
	ENERGY-BAL=YES	Performs energy and mass balance calculations (Default)
FREE-WATER	**FREE-WATER=YES**	Performs free-water calculations
	FREE-WATER=NO	Does not perform free-water calculations (Default)
RESTART	**RESTART=YES**	Uses results from previous convergence pass as initial estimate for next pass (Default)
	RESTART=NO	Initializes each pass
REINIT-BLOCKS	List of convergence and unit operation blocks to be reinitialized in the edit run. If REINIT-BLOCKS=ALL, all blocks are reinitialized. (Default=no blocks are reinitialized)	
REINIT-STREAMS	List of streams whose original values are to be restored in the edit run. If REINIT-STREAMS=ALL, all streams are reinitialized. (Default=no streams are reinitialized)	
TLOWER	Lower limit on temperature (Default=10 K)	
TUPPER	Upper limit on temperature (Default=10000 K)	
PLOWER	Lower limit on pressure (Default=0)	
PUPPER	Upper limit on pressure (Default=1 x 10^{10} N/m^2)	
BYPASS-PROP	**BYPASS-PROP=YES**	Does not perform PROP-SET calculations if flash errors occur (Default)
	BYPASS-PROP=NO	Performs PROP-SET calculations, even if flash errors occur

STOIC-MB-CHECK	**STOIC-MB-CHECK= WARNING**	Gives warning messages during input checking if reaction stoichiometry violates mass balance[9]
	STOIC-MB-CHECK= ERROR	Gives error messages during input checking if reaction stoichiometry violates mass balance (Default)[9]
STOIC-MB-TOL	Tolerance used in checking reaction stoichiometry for mass balance (Default=1)[9]	
MASS-BAL-CHECK	**MASS-BAL-CHECK=YES**	Performs mass balance check around each block as the block is executed, and again after simulation is complete (Default)
	MASS-BAL-CHECK=NO	Does not perform mass balance checking
ATM-PRES	Ambient or atmospheric pressure for gauge pressure calculations (Default=101325 N/m^2)[9]	
FLASH-MAXIT	Maximum number of iterations for flash calculations (Default=30)	
FLASH-TOL	Tolerance for flash calculations (Default=$1x10^{-4}$)	
NPHASE	Maximum number of phases in a MIXED substream. Use to override the default for NPHASE in UOS blocks and input paragraphs.[9] See Table 48.2.	
	NPHASE=1	One-phase calculation
	NPHASE=2	Two-phase calculation
	NPHASE=3	Three-phase calculation
PHASE	Specifies the phase when NPHASE=1. Use to override the default for PHASE in UOS blocks and input paragraphs.[9] See Table 48.2.	
	PHASE=V	Vapor (Default)
	PHASE=L	Liquid
PARADIGM	Specifies the flowsheet solution mode.	
	PARADIGM=SM	Use the traditional block-by-block sequential modular approach to solve the flowsheet (Default)
	PARADIGM=EO	Use the new equation-oriented approach to solve the whole flowsheet simultaneously after initializing the flowsheet with sequential modular approach. See Chapter 48 for Equation-Oriented Solution.
	PARADIGM=MIXED	This is a hybrid of the two options above. In the MIXED mode, you can solve hierarchies with equation-oriented approach but solve the whole flowsheet with sequential modular approach. You specify the solution method of a hierarchy and its subhierarchies with the SOLVE paragraph in Chapter 48. Note that the solution method of the SOLVE paragraph is only used when PARADIGM=MIXED is enabled. Also note that EO hierarchies are always solved in the simulation mode.

9 This keyword only affects the block used and value entered in the edit run.

Table 47.2 Overriding Defaults for NPHASE and PHASE

UOS Model/Input Paragraph	Sentences	Keywords
STREAM	—	NPHASE, PHASE
MIXER	PARAM	NPHASE, PHASE
FSPLIT	PARAM	NPHASE, PHASE
SSPLIT	PARAM	NPHASE, PHASE
SEP	PARAM	NPHASE, PHASE
	FLASH-SPECS	NPHASE, PHASE
SEP2	PARAM	NPHASE, PHASE
	FLASH-SPECS	NPHASE, PHASE
HEATER	PARAM	NPHASE, PHASE
FLASH2	PARAM	NPHASE†
HEATX	FLASH-SPECS	NPHASE, PHASE
MHEATX	HOT-SIDE	NPHASE, PHASE
	COLD-SIDE	NPHASE, PHASE
RSTOIC	PARAM	NPHASE, PHASE
RYIELD	PARAM	NPHASE, PHASE
REQUIL	PARAM	NPHASE, PHASE††
RGIBBS	PARAM	NPHASE, VAPOR†††
RCSTR	PARAM	NPHASE, PHASE
RPLUG	PARAM	NPHASE, PHASE
COOLANT	PARAM	NPHASE, PHASE
RBATCH	PARAM	NPHASE, PHASE, NPHASE-ACCUM, PHASE-ACCUM
PUMP	PARAM	NPHASE
COMPR	PARAM	NPHASE
MCOMPR	PARAM	COMPR-NPHASE, COOLER-NPHASE
PIPELINE	PARAM	NPHASE, PHASE
PIPE	PARAM	NPHASE, PHASE
VALVE	PARAM	NPHASE, PHASE
CRYSTALLIZER	PARAM	NPHASE
USER	FLASH-SPECS	NPHASE, PHASE
USER2	FLASH-SPECS	NPHASE, PHASE
CALCULATOR	FLASH-SPECS	NPHASE, PHASE
TRANSFER	FLASH-SPECS	NPHASE, PHASE
BALANCE	FLASH-SPECS	NPHASE, PHASE
PROP-TABLE		
FLASHCURVE	PARAM	NPHASE†
RESIDUE	PARAM	NPHASE†
PRES-RELIEF	PARAM	NPHASE, VENT-NPHASE, VENT-PHASE

† If NPHASE is set to 1 in SIM-OPTIONS, the local NPHASE is set to 2.

†† If NPHASE is set to 3 in SIM-OPTIONS, the local NPHASE is set to 2.

††† In SIM-OPTIONS, if NPHASE is set to 1 and PHASE is set to L, the local VAPOR is set to NO.

DELETE Paragraph

Input Language for DELETE

```
DELETE
BLOCK    blockid-list
CALCULATOR    cblockid-list
CASE-STUDY
CONSTRAINT    conid-list
CONVERGENCE    cvblockid-list
CONV-ORDER
DATA-SET    datasetid-list
DESIGN-SPEC    specid-list
OPTIMIZATION    optid-list
PRES-RELIEF    pblockid-list
PROFILE-DATA    profdataid-list
PROP-TABLE    tableid-list
REGRESSION    rblockid-list
REPORT-SCALE
SENSITIVITY    sblockid-list
SEQUENCE    seqid-list
STREAM    sid-list
TEAR    sid-list
TRANSFER    tblockid-list
```

Input Language Description for DELETE

Use the DELETE paragraph to remove paragraphs from the previous run. The DELETE paragraph is hierarchical, but in each DELETE paragraph you can only delete paragraphs in the same hierarchy.

BLOCK Use to delete unit operation blocks from the flowsheet. When a unit operation block is deleted, use the FLOWSHEET paragraph to describe the modified flowsheet connectivity that results. After unit operation blocks are deleted, Aspen Plus automatically deletes any streams that have no source block and no destination block. Aspen Plus also automatically deletes any design specifications, CALCULATOR blocks, TRANSFER blocks, SENSITIVITY blocks, CASE-STUDY blocks, constraints, optimization problems, or REPORT-SCALE paragraphs referencing deleted blocks or streams.

blockid-list..... List of unit operation blocks (BLOCK paragraphs) to be deleted from the flowsheet

CALCULATOR Use to delete CALCULATOR blocks.

cblockid-list ..... List of CALCULATOR blocks

CASE-STUDY Use to delete the CASE-STUDY paragraph.

CONSTRAINT Use to delete CONSTRAINTs. (See Note 1.)

conid-list..... List of CONSTRAINTs to be deleted

CONVERGENCE Use to delete CONVERGENCE blocks. You must delete any CONV-ORDER paragraphs referencing these blocks. CONV-ORDER paragraphs are not deleted automatically. (See Note 3.)

cvblockid-list ..... List of CONVERGENCE blocks

CONV-ORDER Use to delete user-specified convergence order.

DATA-SET Use to delete data-fit DATA-SET paragraphs.

	datasetid-list ..... List of DATA-SET ID paragraphs
DESIGN-SPEC	Use to delete DESIGN-SPEC paragraphs.
	specid-list ..... List of DESIGN-SPEC paragraphs. (See Note 2.)
OPTIMIZATION	Use to delete optimization problems. (See Notes 1 and 2.)
	optid-list ..... List of optimization problems
PRES-RELIEF	Use to delete PRES-RELIEF blocks.
	pblockid-list ..... List of pressure relief blocks
PROFILE-DATA	Use to delete PROFILE-DATA paragraphs.
	profdataid-list ..... List of PROFILE-DATA paragraphs
PROP-TABLE	Use to delete PROP-TABLE paragraphs. You must delete any PROP-TABLE paragraphs that reference deleted streams. PROP-TABLE paragraphs are not deleted automatically.
	tableid-list ..... List of PROP-TABLE paragraphs
REGRESSION	Use to delete data-fit REGRESSION paragraphs.
	rblockid-list ..... List of REGRESSION paragraphs
REPORT-SCALE	Use to delete the REPORT-SCALE paragraphs.
SENSITIVITY	Use to delete SENSITIVITY blocks.
	sblockid-list ..... List of SENSITIVITY blocks
SEQUENCE	Use to delete user-specified SEQUENCE paragraphs. You must delete any SEQUENCE paragraphs containing deleted unit operation blocks, CALCULATOR blocks, SENSITIVITY blocks, CONVERGENCE blocks, TRANSFER blocks, PRES-RELIEF blocks, REGRESSION blocks, or another SEQUENCE paragraph that is deleted. SEQUENCE paragraphs are not deleted automatically.
	seqid-list..... List of SEQUENCE paragraphs
STREAM	Use to delete your selected streams from the flowsheet and unit operation blocks. Aspen Plus automatically deletes any streams that have no source block and no destination block.
	sid-list ..... List of stream IDs to be deleted from the flowsheet and unit operation blocks
TEAR	Use to delete user-specified tear streams. CONVERGENCE blocks that converge deleted tear streams will be automatically deleted.
	sid-list ..... List of TEAR streams
TRANSFER	Use to delete transfer blocks.
	tblockid-list ..... List of transfer blocks

SIMULATE and NOSIMULATE Paragraphs

Input Language for SIMULATE and NOSIMULATE

```
SIMULATE    [START=blockid]    [STOP=blockid]
NOSIMULATE
```

Input Language Description for SIMULATE and NOSIMULATE

Use the SIMULATE paragraph to execute only a selected part of the calculation sequence. Use the NOSIMULATE paragraph to indicate that no simulation calculations are to be performed.

START	First block to be executed. (Default=beginning of calculation sequence.) Can be hierarchical; see Chapter 9 for naming conventions and restrictions.
STOP	Last block to be executed. (Default=end of calculation sequence.) Can be hierarchical; see Chapter 9 for naming conventions and restrictions.

Notes

1. When you replace or delete a CONSTRAINT in an edit run, you should also replace the OPTIMIZATION paragraph that references the CONSTRAINT. When you delete an OPTIMIZATION paragraph, you must delete all CONSTRAINTs referenced by the OPTIMIZATION.
2. When you replace or delete a DESIGN-SPEC or OPTIMIZATION paragraph in an edit run, and that DESIGN-SPEC or OPTIMIZATION paragraph is referenced by a user-specified CONVERGENCE block, you must replace or delete the CONVERGENCE block in the edit run. System-defined CONVERGENCE blocks are automatically deleted.
3. When you delete a CONVERGENCE block, you should also use a DELETE paragraph to delete any tear streams associated with that block. When you replace a CONVERGENCE block in an edit run, and change the set of tear streams converged by that block, you should also use a DELETE paragraph to delete the streams that are no longer torn.

Running an Edit Run Input File

The command used to run an edit run input file is similar to that described in the ASPEN run command, Chapter 2. The ASPEN run command is case insensitive.

```
ASPEN input_file [runid]
```

Where:

input_file	=	A file written in Aspen Plus input language that defines the paragraphs to be added, modified, or deleted. (See Table 48.1.) The default file type is .inp and does not need to be included in the command line.
runid	=	Identifier for the previous simulation program to be edited. The runid must have the file type .appdf. You must always specify this parameter for EDIT runs. To maintain your previous simulation results, you must copy your original simulation files into a separate set of identifiers.

48 Equation-Oriented Simulation

This chapter describes the input language for Equation-Oriented paragraphs. All of them, except for GLOBALSCRIPT, can be entered at the Plant level or the Hierarchy level.

The following paragraphs are descibed in this chapter:

- **EO-OPTIONS** – Set options for the EO Configuration.
- **INIT-VAR-ATTR** – Change open variable attributes.
- **EO-PORT** – Define the variables that make up a port.
- **SPECGROUPS** – Define variables in a SpecGroup and set their specifications.
- **EOSENSITIVITY** – Configure the set of independent and dependent EO variables for sensitivity analysis.
- **LOCALSCRIPT** – Define local scripts.
- **GLOBALSCRIPT** – Define global scripts.
- **SCRIPTMETHOD** – Define script methods.
- **EO-CONV-OPTI** – Specify Equation-Oriented convergence parameters.
- **SOLVE** – Specify SM or EO solution and EO run mode.

EO-OPTIONS Paragraph

Input Language for EO-OPTIONS

```
EO-OPTIONS
PARAM    keyword=value
```

Keywords:

COMPS EO-FORM SPARSITY LIGHT-KEY HEAVY-KEY DEP-COMPS DERIV-METHOD SOLVE-METHOD CHECK-FREE-W PASS-THROUGH NEG-COMP-CHK NEG-FLOW-CHK INLET-PHASE FLASH-FORM L2-COMP-MODE L2-COMP VFRACX-TOL VFRAC-TOL FLOW-TOL ON-SMEO-DIFF MIN-PRES PRES-TOL AUTO-COMPS AUTO-COMPS-T AUTO-PHASE AUTO-PHASE-T

```
MODEL-OPTION  modeltype  keyword=value
```

Keywords:

COMPS EO-FORM SPARSITY LIGHT-KEY HEAVY-KEY DEP-COMPS DERIV-METHOD SOLVE-METHOD CHECK-FREE-W PASS-THROUGH NEG-COMP-CHK NEG-FLOW-CHK INLET-PHASE FLASH-FORM L2-COMP-MODE L2-COMP VFRACX-TOL VFRAC-TOL FLOW-TOL ON-SMEO-DIFF MIN-PRES PRES-TOL AUTO-COMPS AUTO-COMPS-T AUTO-PHASE AUTO-PHASE-T

```
SECTION-OPTI  sectionid  keyword=value
```

Keywords:

COMPS EO-FORM SPARSITY LIGHT-KEY HEAVY-KEY DEP-COMPS DERIV-METHOD SOLVE-METHOD CHECK-FREE-W PASS-THROUGH NEG-COMP-CHK NEG-FLOW-CHK INLET-PHASE FLASH-FORM L2-COMP-MODE L2-COMP VFRACX-TOL VFRAC-TOL FLOW-TOL ON-SMEO-DIFF MIN-PRES PRES-TOL AUTO-COMPS AUTO-COMPS-T AUTO-PHASE AUTO-PHASE-T

Input Language Description for EO-OPTIONS

PARAM Use to specify equation-oriented options at the plant or hierarchy level. See below for keywords.

MODEL-OPTION Use to specify equation-oriented options for all instances of a model type. See below for keywords.

modeltype..... UOS model type, such as FLASH2 or MIXER.

SECTION-OPTI Use to specify equation-oriented options for a flowsheet section. See below for keywords.

sectionid..... Flowsheet section id.

The following keywords are used for the PARAM, MODEL-OPTION, and SECTION-OPTI sentences.

COMPS..... Component group for a list of components which can be active in the plant or hierarchy

EO-FORM..... Equation-oriented formulation

EO-FORM=STANDARD	Standard formulation. Compositions in terms of mole fractions. Stream variables named using Aspen Plus stream names.(Default)
EO-FORM=EOPML	For RT-Opt 10.0 / DMO compatibility. Compositions in terms of mole fractions. Stream variables named using PML convention.
EO-FORM=MOLEFRAC	For RT-Opt 10.0 compatibility. Compositions in terms of molar fractions. Stream variables named using PML convention. Some reduced functionality.
EO-FORM=MOLEFLOW	For RT-Opt 3.0 compatibility. Compositions in terms of molar flows. Stream variables named using Aspen Plus stream names.

SPARSITY ..... Used to set the dependence of thermodynamic properties on state variables and compositions while evaluating derivatives.

SPARSITY=FULL	Temperature, pressure and composition dependence
SPARSITY=COMP-INDEP	Temperature and pressure dependence
SPARSITY=WATER-SOLU	Temperature, pressure and composition dependence for water, temperature and pressure dependence for all other components

LIGHT-KEY ..... Component ID of the lightest distributing component

HEAVY-KEY ..... Component ID of the heaviest distributing component

DEP-COMPS ..... Component group of components for which fugacities are composition-dependent. Pure component fugacities are used for all other components.

DERIV-METHOD ..... Preferred derivatives method, Analytic or Numeric. Update methods should not be used for Degree of Freedom run modes (Optimization or Reconciliation).

DERIV-METHOD = ANALYTICAL	Model derivatives (Jacobian) are determined from coded analytic expressions. Generally the preferred method. (Default)
DERIV-METHOD = NUMERICAL	Alternate method for calculating Jacobian. Useful when there is concern that analytic derivatives are causing convergence difficulties. Usually slower than analytic derivatives, more subject to precision issues.
DERIV-METHOD = UPDATE-ANALY	Use Schubert method for updating Jacobian, with analytic derivatives for Base Jacobian. Use when Jacobian calculation is rate limiting step. May result in more iterations and be less robust than calculated derivatives.
DERIV-METHOD = UPDATE-NUMER	Use Schubert method for updating Jacobian, with numerical derivatives for Base Jacobian. Use when Jacobian calculation is rate limiting step. May result in more iterations and be less robust than calculated derivatives.

SOLVE-METHOD ..... EO solution method. Specifies if open, closed, or neither method should be used with desired action and message level on failure.

SOLVE-METHOD = OPEN-PERT-IN	Open solution method; on failure use Perturbation with information messages. (Default for most blocks)
SOLVE-METHOD = OPEN-PERT-WA	Open solution method; on failure use Perturbation with warning messages.
SOLVE-METHOD = OPEN-NOPERT	Open solution method; on failure stop with error messages.

	SOLVE-METHOD= PERTURBATION	Closed solution method; use Perturbation layer around closed model. (Default for Design-Spec blocks)
	SOLVE-METHOD= DO-NOT-CREAT	Ignore during EO solution.

CHECK-FREE-W ..... Check if only water appears in a stream when Free-Water=Yes. If so, turn off Free-Water in VLE calculations, and do not consider the existence of any other components.

CHECK-FREE-W = YES	Check for presence of only water (Default)
CHECK-FREE-W = NO	Do not check for presence of only water

PASS-THROUGH ..... Forces an APStrm model to be in pass-through mode, creating both input and output streams.

PASS-THROUGH = YES	Create both input and output streams
PASS-THROUGH = NO	Do not create both input and output streams (Default)

NEG-COMP-CHK ..... Negative composition check/Value used to check for negative mole fractions and issue warnings during the report phase. (Default=-$1x10^{-8}$)

NEG-FLOW-CHK ..... Negative flow check/Value used to check for negative mole flow and issue warnings during the report phase. (Default=0.0)

INLET-PHASE ..... Phase for the Material port. If unspecified, the phase will be obtained from the upstream conditions.

INLET-PHASE = V	Vapor only
INLET-PHASE = L	Liquid only
INLET-PHASE = MIXED	Vapor-Liquid or Vapor-Liquid-FreeWater depending on the block's free-water option

ON-SMEO-DIFF ..... Indicates action to take in certain cases where the EO results differ from the SM results. This applies in overspecified FSplit, RStoic, RYield, Sep, and Sep2 blocks when the SM run renormalizes the specifications; the EO model uses the renormalized specifications based on conditions at initialization, though the conditions may change at the final solution. This also applies in HeatX blocks with phase-dependent heat transfer coefficients if the phase changes between initialization and solution conditions.

ON-SMEO-DIFF = USE-CLOSED	Use the result from SM calculations. (Default)
ON-SMEO-DIFF = USE-OPEN	Use the result from EO calculations.

AUTO-COMPS ..... Specifies in which situations to automatically reduce the component slate by removing missing components. When active, this option removes from the component list for this block the components whose mole fractions are less than AUTO-COMPS-T. Additional checks are made around models with reactions and user models.

AUTO-COMPS = ALWAYS	Always remove missing components.
AUTO-COMPS = IF-NO-COMPS	Remove missing components if non-zero components were *not* specified through the COMPS keyword. (Default)
AUTO-COMPS = NEVER	Never remove missing components.

AUTO-COMPS-T ..... Tolerance used with AUTO-COMPS. Components with mole fractions less than this value are removed from the block when AUTO-COMPS is active. (Default 0.)

The following keywords are used for the PARAM, MODEL-OPTION, and SECTION-OPTI sentences, but apply only to the blocks which can perform

flashes in EO: Stream, Analyzer, Flash2, Flash3, FSplit, Heater, HeatX, Mixer, Pump, RStoic, RYield, Sep, and Sep2.

FLASH-FORM ..... Flash formulation.

FLASH-FORM = PML	The original EO flash formulation, supporting two-phase and two-phase-free-water flashes. (Default for two-phase and two-phase-free-water flashes.)
FLASH-FORM = SMOOTHING	The smoothing flash uses a smoothing function for the phase fractions near the phase boundary. The parameters VFRACX-TOL and VFRAC-TOL affect the accuracy of this function. (Default for three-phase flashes.)

L2-COMP-MODE ..... Method of choosing a key component for a three-phase flash. In FLASH3, the key component is specified via the block's L2-COMP keyword and this keywords is not used.

L2-COMP-MODE = AUTO	Aspen Plus chooses a component. (Default)
L2-COMP-MODE = NONE	A key component is not chosen.
L2-COMP-MODE = COMPID	One or more components are specified with the L2-COMP keyword.

L2-COMP ..... List of component IDs as the key components for a three-phase flash. Used only when L2-COMP-MODE is COMPID. Not used in FLASH3.

VFRACX-TOL ..... Smoothing tolerance for the extended vapor fraction used in the two-phase free-water flash and the three-phase flash when the FLASH-FORM is SMOOTHING. (Default 10^{-5})

VFRAC-TOL ..... Smoothing tolerance for the phase fractions used in the two-phase free-water flash and the three-phase flash when the FLASH-FORM is SMOOTHING. Reducing this value improves the accuracy of the flash near the phase boundaries, but makes the problem more non-linear. (Default 10^{-3})

FLOW-TOL..... Smoothing tolerance for preventing molar flows from becoming zero, used in the two-phase free-water flash and the three-phase flash when the FLASH-FORM is SMOOTHING. Used only in the Heater and HeatX models for computing the pressure drop parameter. (Default 10^{-4} kmol/s)

MIN-PRES ..... Determines which system is used to handle pressure drop specifications in blocks with multiple inlet streams.

MIN-PRES = YES	A smoothing function is applied repeatedly to the pressures of the inlet streams in order to determine the minimum inlet pressure. (Default)

$$\min(X_1, X_2) = \tfrac{1}{2}\left[\left(X_1 + X_2\right) + \sqrt{\left(X_1 - X_2\right)^2 + \beta^2}\right]$$

MIN-PRES = NO	The inlet stream with lowest inlet pressure at initialization has its pressure drop made Constant. May lead to problems if another inlet stream subsequently has a lower pressure. Used for compatibility with Aspen Plus 11.1.

PRES-TOL..... Smoothing tolerance β in smoothing function for calculating minimum inlet pressure. The smoothing tolerance must be small enough to maintain accuracy but not so small as to create numerical difficulties, and the default is reasonable for most applications.

AUTO-PHASE..... Specifies in which situations to automatically reduce the phases in the block by eliminating missing ones. This applies to all flashes in the block (outlet, mixed inlet, and dew or bubble point flashes). When active, this option removes from the allowed phases for this block any phases whose extended phase fractions are beyond the range of 0 to 1 by more than AUTO-PHASE-T. This tolerance avoids the problems encountered by removing phases near the bubble or dew point.

AUTO-PHASE will also drop any phases for which the flash algorithm fails to converge on the phase compositions, and will drop one liquid phase in three-phase calculations if the two liquid compositions are identical.

AUTO-PHASE = YES	Remove missing phases. (Default)
AUTO-PHASE = NO	Do not check for missing phases.

AUTO-PHASE-T ..... Tolerance used with AUTO-PHASE. Phases with extended phase fractions are beyond the range of 0 to 1 by more than this value are removed from the block when AUTO-PHASE is active. (Default 0.1.)

INIT-VAR-ATTR Paragraph

Input Language for INIT-VAR-ATTR

```
INIT-VAR-ATTR
INITIALIZE vname keyword=value
```

Optional keywords:

VALUE LOWER UPPER STEP BOUND-TYPE SBWEIGHT PHYS-QTY UOM SCALE

Input Language Description for INIT-VAR-ATTR

INITIALIZE Use to specify the attributes of open variables.

vname..... Name of the open variable (Required)

VALUE..... Current value of the variable

LOWER..... Lower bound

UPPER..... Upper bound

STEP ..... Step bound

BOUND-TYPE ..... Bound type

BOUND-TYPE = HARD	Do not violate the upper and/or lower bounds when solving a non-square (optimization or data regression) problem. (Default)
BOUND-TYPE = RELAXED	Relax upper and/or lower bound. If the initial value is outside the bound, set the bound to the initial value.
BOUND-TYPE = SOFT	Same as relaxed but add a penalty term to the objective to try to drive the value back to the bound.

SBWEIGHT..... Soft bound weight

PHYS-QTY..... The physical quantity that the variable represents, for example, mole flow, temperature, or pressure. These types correspond to the standard Aspen Plus types.

UOM..... Units of measure (standard Aspen Plus units), based on the physical type of the variable. Internally, all values are stored in SI units.

SCALE ..... Scale factor used by the solver

EO-PORT Paragraph

Input Language for EO-PORT

```
EO-PORT portid
EO-PORT keyword=value
```

Optional keywords:

VAR VALUE TYPE COMPONENTS THRU PHASE PHYS-QTY UOM

Input Language Description for EO-PORT

EO-PORT

Use to define the variables that make up a port. A port is an arbitrary collection of variables. Ports can make connecting groups of variables easier.

VAR ..... Open variable name

VALUE ..... Initial value

TYPE ..... Type of port

TYPE = MOLE-FLOW	Material stream (flow basis)
TYPE = MOLE-FRAC	Material stream (fraction basis)
TYPE = HEAT	Heat stream
TYPE = WORK	Work stream
TYPE = GENERIC	Generic collection

COMPONENTS ..... Comp-Group ID. Correction for the component list if the global component list is not being used.

THRU ..... Whether to include all variables from VAR in this EO-PORT sentence through VAR in the next EO-PORT sentence.

THRU = YES	Include all variables.
THRU = NO	Do not include all variables. (Default)

PHASE ..... Phase for the material port. If unspecified, the phase will be obtained from the upstream conditions.

PHASE = V	Vapor only
PHASE = L	Liquid only
PHASE = VL	Vapor and Liquid
PHASE = VLW	Vapor, Liquid, and Free-Water

PHYS-QTY ..... The physical quantity that the variable represents, for example, mole flow, temperature, or pressure. These types correspond to the standard Aspen Plus types.

UOM ..... Units of measure (standard Aspen Plus units), based on the physical type of the variable. Internally, all values are stored in SI units.

SPECGROUPS Paragraph

Input Language for SPECGROUPS

```
SPECGROUPS
SPEC-GROUP specgroupid keyword=value
```

Optional keywords:

ENABLED COMMENT

```
SPEC-CHANGE specgroupid keyword=value
```

Optional keywords:

VAR SPEC

Input Language Description for SPECGROUPS

SPEC-GROUP

Use to override default variable specifications. Each spec group must not change the net specification of the problem.

specgroupid ..... Spec group name

ENABLED..... Whether the spec group is enabled or disabled

ENABLED = YES	Spec group is enabled (Default)
ENABLED = NO	Spec group is disabled

COMMENT ..... Optional comment associated with the spec group

SPEC-CHANGE

Use to add a variable to a spec group.

specgroupid ..... Spec group name

VAR..... Open variable name

SPEC ..... Change applied by the user to change the initial specification

SPEC = CALC	Calculated
SPEC = CONST	Constant
SPEC = INDEP	Independent
SPEC = MEAS	Measured
SPEC = PARAM	Parameterized
SPEC = OPTIM	Optimized
SPEC = RECON	Reconciled

EOSENSITIVITY Paragraph

Input Language for EOSENSITIVITY

```
EOSENSITIVITY sensitivityid
PARAM keyword=value
```

Optional keywords:

OBJECTIVE EVALJCBN FORCESPECS

```
LIST keyword=value
```

Optional keywords:

INDEPVAR DEPVAR

Input Language Description for EOSENSITIVITY

PARAM Use to specify optional parameters.

OBJECTIVE..... Optional ID of an objective function. If specified, the sensitivity of the objective to the independent variables is calculated.

EVALJCBN ..... Do/Do not evaluate the Jacobian before calculating sensitivity.

EVALJCBN = YES	Evaluate the Jacobian (Default)
EVALJCBN = NO	Do not evaluate the Jacobian

FORCESPECS..... Whether to force variable specifications in the INDEPVAR and DEPVAR lists

FORCESPECS = YES	Force the specifications (Default)
FORCESPECS = NO	Do not force the specifications

LIST Use to list the independent and dependent variables for sensitivity analysis

INDEPVAR..... List of independent variables. The selected variables must be fixed or a degree of freedom in the current mode.

DEPVAR ..... List of dependent variables. The selected variables must be free in the current mode.

LOCALSCRIPT Paragraph

Input Language for LOCALSCRIPT

```
LOCALSCRIPT scriptid
SCRIPT "any amount of text entered on any number of lines and enclosed in
       double quotes"
```

Input Language Description for LOCALSCRIPT

SCRIPT Use to enter the script lines

GLOBALSCRIPT Paragraph

Input Language for GLOBALSCRIPT

```
GLOBALSCRIPT scriptid
SCRIPT "any amount of text entered on any number of lines and enclosed in
       double quotes"
```

Input Language Description for GLOBALSCRIPT

SCRIPT Use to enter the script lines

SCRIPTMETHOD Paragraph

Input Language for SCRIPTMETHOD

```
SCRIPTMETHOD
SCRIPTS keyword=value
```

Keywords:

METHOD TYPE LOCALSCRIPT GLOBALSCRIPT FILE

Input Language Description for SCRIPTMETHOD

SCRIPTS Any number of SCRIPTS sentences may be entered. Each one describes a new METHOD.

METHOD ..... Name of a script method

TYPE ..... Type of script

TYPE = LOCALSCRIPT	If entered, LOCALSCRIPT must be specified.
TYPE = GLOBALSCRIPT	If entered, GLOBALSCRIPT must be specified.
TYPE = FILE	If entered, FILE must be specified.

LOCALSCRIPT ..... ID of a LOCALSCRIPT paragraph

GLOBALSCRIPT ..... ID of a GLOBALSCRIPT paragraph

FILE ..... Name of a file

EO-CONV-OPTI Paragraph

Input Language for EO-CONV-OPTI

```
EO-CONV-OPTI
PARAM keyword=value
```

Optional Keywords:

SOLVER

```
SM-INIT keyword=value
```

Optional keywords:

MAXIT WAIT NACCELERATE PRINT-LEVEL QMIN QMAX MAXIPASS TOLINI SKIP-INIT MAXFITER

```
DMO-PARAMS mode keyword=value
```

Optional keywords:

RESCVG OBJCVG MAXITER MINITER CREEPFLAG CREEPITER CREEPSIZE PRINTLEVEL PRINTFREQ SCREENFORM SEARCHMODE HESSIANSCL HESSIANUPD LINESEARCH LINESRCMODE LSMODEITER VARSCALE TRUSTMODE TRUSTITER TRUSTRAMPIT TRUSTSIZE ADCVMETH ADCVITER ADCVOBJCVG ADCVRESCVG QPMICROINF QPMICROTOL QPMICROMAX QPSTATS QPDEPDIAGS ACTIVERPT BOUNDRPT IPSIRPT ACTIVESAVE ACTIVEINIT RIGORUPD QPITER QPHESSIANUPD QPCONVTOL USEDROPTOL DROPTOL PIVOTSEARCH PIVOTANAL ANALTHRESH PIVOTTHRESH PIVOTZERO FACTORSPEED BTF MINBTFSIZE DENSITYRATIO SINGULARHAND LUSTATS FREEONLY FACTORSPACE ACTIVESPACE IWORKF RWORKF CWORKF

```
LSSQP-PARAMS mode keyword=value
```

Optional keywords:

RELEPS RFEASB RFINFB MAXITER MINITER MAXLSF MAXQPF NFEASB NFINFB KPTLEV KPLLEV KPFREQ KPNTOP MDHESS TAUHYB LSCOPT TRBND CHGBND CHGMAX BNDAPP INICHK LSIZEB1 LSIZEB2 FSCALF ETASKP RRLOW RRHIGH BSMALL ZPERTF IFDTYP IFDITER IFDFREQ DELTLS MAXLSC ALFALS IXSCS BIGSCL SMLSCL KMUDEC VMUINI VMUMIN VMUFAC KFOWDG KBKOUT LEWBAS BNDADJ GNPMAX QPINFE SPDROP NCSRCH SINGT1 SINGT2 TOLBAS TOLANA LCHBAS NBDBAS BASFLP MSMETH MSFREQ NUMDER DPERTF XPMIN DERDIF DERMIN LUBNDS BIGBND LINCST NNDCMP

Input Language Description for EO-CONV-OPTI

PARAM Use to specify the EO solver.

SOLVER..... Lets you specify which EO solver to use

SOLVER = DMO	Use the DMO solver (Default)
SOLVER = LSSQP	Use the LSSQP solver

SM-INIT Use to specify the sequential-modular (SM) initialization parameters at the hierarchical block and flowsheet levels.

MAXIT ..... Maximum number of flowsheet evaluations (Default=3)

WAIT ..... Number of direct substitution iterations before the first acceleration iteration (Default=2)

NACCELERATE ..... Number of consecutive acceleration iterations (Default=2)

PRINT-LEVEL ..... Level of errors and diagnostics printed in the history file (Default from DIAGNOSTICS paragraph)

QMIN ..... Lower bound for the Wegstein acceleration parameters (q) (Default=–5.0)

QMAX ..... Upper bound for the Wegstein acceleration parameters (q) (Default=0.9)

MAXIPASS ..... Maximum number of sequential-modular initialization passes (Default=2)

TOLINI ..... Tolerance for sequential-modular initialization (Default=$1x10^{-3}$)

SKIP-INIT ..... Skip sequential-modular initialization if block and streams have been previously initialized (Default=YES)

SKIP-INIT = NO	Do not skip initialization
SKIP-INIT = YES	Skip initialization

MAXFITER ..... Maximum number of iterations after failure of equation-oriented solution, to switch back to sequential-modular (Default=2)

DMO-PARAMS

Use to specify parameters for controlling the accuracy, performance, and robustness of the DMO solver.

mode ..... Run mode.

mode = DEFAULT	Default for all run modes
mode = SIM	Simulation mode
mode = PARAM	Parameter estimation mode
mode = RECON	Data reconciliation mode
mode = OPTIM	Optimization mode

RESCVG ..... Residual convergence tolerance (Default=$1x10^{-6}$)

OBJCVG ..... Objective function convergence tolerance (Default=$1x10^{-6}$)

MAXITER ..... Maximum number of SQP iterations allowed (Default=50)

MINITER ..... Minimum number of SQP iterations allowed (Default=0)

CREEPFLAG ..... Creep mode. This mode is very effective for making the optimizer moves more conservative. It is particularly helpful when the problem diverges

CREEPFLAG = ON	Use creep mode
CREEPFLAG = OFF	Do not use creep mode (Default)

CREEPITER ..... Number of iterations to perform creep mode (Default=10)

CREEPSIZE ..... Creep mode step size, as a fraction of the full step size when in creep mode (Default=0.1)

PRINTLEVEL ..... Diagnostic printing level for variables and residuals

PRINTLEVEL = **BRIEF**	Print 10 worst residuals (Default)
PRINTLEVEL = **FULL**	Print all variables & residuals. **Warning:** Using the Full option can result in very large amounts of output.

PRINTFREQ ..... Diagnostic printing frequency for variables and residuals. Print variables & residuals at every nth iteration. (Default=1)

SCREENFORM ..... Output for the iteration log. File output shows more significant figures than terminal output.

SCREENFORM = **FILE**	Print to file
SCREENFORM = **TERMINAL**	Print to terminal (Default)

SEARCHMODE ..... Hessian initialization mode

SEARCHMODE = AGGRESSIVE	Hessian initialized with small values. Moves problem to bounds faster than Normal mode. Preferred for highly constrained optimization problems with few DOF at solution. Ideal applications are well-posed online real-time optimization problems.
SEARCHMODE = NORMAL	Hessian initialized with identity matrix. Balances efficiency and robustness. Well suited for general-purpose optimization problems. Typical applications are offline optimization or online problems that start very far from soln.
SEARCHMODE = **ADVANCED**	Hessian initialized with 2nd order information. Recommended for problems with many degrees of freedom at solution and/or quadratic objective function. Ideal for data reconciliation problems (both online and offline). (Default)
SEARCHMODE = **SCALED**	Combination of the Aggressive and Advanced modes. Recommended for highly constrained optimization problems with few degrees of freedom at solution and nonlinear objective function.

HESSIANSCL ..... Used defined factor for scaling the identity matrix. Used with Scaled Hessian initialization mode only. (Default=1)

HESSIANUPD ..... Number of Hessian updates stored before reinitializing (Default=10)

LINESEARCH ..... Line search algorithm

LINESEARCH = 0	The well known exact penalty line search. It is too conservative for most practical problems.
LINESEARCH = 2	A proprietary line search designed to initially favor the convergence of residuals over the objective function improvement
LINESEARCH = 3	A proprietary line search designed to balance robustness with efficiency (Default)
LINESEARCH = 4	A line search designed to attempt enforcing bounds on cases with no degrees of freedom. It should be used only in cases where there are multiple solutions to a problem and the desired one lies within the bounds.

LINESRCMODE ..... Line search mode for step control.

LINESRCMODE = NORMAL	Original method (Default)
LINESRCMODE = AGGRESSIVE	Modified method that tends to take larger steps
LINESRCMODE = CONSERVATIVE	Modified method that tends to take smaller step

LSMODEITER..... Number of iterations to perform step control. 0 for Normal step control mode; > 0 for Aggressive or Conservative step control mode. Default depends on selected step control mode: 0 for Normal, 5 otherwise.

VARSCALE..... Whether to use variable scaling

	VARSCALE = ON	Use variable scaling (Default)
	VARSCALE = OFF	Do not use variable scaling
TRUSTMODE	This switch enables the application of a trust region that will limit the optimization moves for the OPTIM variables only. The size is specified as a fraction of the original variable bound range.	
	TRUSTMODE = ON	Use trust mode
	TRUSTMODE = OFF	Do not use trust mode (Default)
TRUSTITER	The number of iterations the trust region will be applied with a fixed size (Default=2)	
TRUSTRAMPIT	The number of iterations, following the fixed iterations, over which the size of the trust region is gradually increased until it reaches the original variable bound range (Default=2)	
TRUSTSIZE	This is the range that the OPTIM variables are initially allowed to move (for all the fixed iterations), expressed as a fraction of the original variable bound range (Default=0.1)	
ADCVMETH	Method for terminating the optimization moves while closing any remaining residuals	
	ADCVMETH = NONE	Do not terminate optimzation moves (Default)
	ADCVMETH = ANY	Terminate if threshold specified in ADCVITER, ADCVOBJCVG, or ADCVRESCVG is reached.
	ADCVMETH = ITERATIONS	Terminate if threshold specified in ADCVITER is reached.
	ADCVMETH = OBJECTIVE	Terminate if threshold specified in ADCVOBJCVG is reached.
	ADCVMETH = RESIDUAL	Terminate if threshold specified in ADCVRESCVG is reached.
	ADCVMETH = ALL	Terminate if thresholds specified in ADCVITER, ADCVOBJCVG, and ADCVRESCVG are reached.
ADCVITER	Number of iterations before activating the advanced convergence method (Default=100)	
ADCVOBJCVG	Objective function convergence tolerance threshold before activating the advanced convergence method (Default=$1x10^{-6}$)	
ADCVRESCVG	Residual convergence tolerance threshold before activating advanced convergence method (Default=$1x10^{-6}$)	
QPMICROINF	Flag controlling the automatic micro-infeasibility handling in the QP.	
	QPMICROINF = ON	Turn flag on
	QPMICROINF = OFF	Turn flag off (Default)
QPMICROTOL	Absolute relaxation of an infeasible bound in the QP when micro-infeasibility handling is enabled (Default=$1x10^{-12}$)	
QPMICROMAX	Maximum number of micro-infeasibility handling attempts that can be done in one DMO iteration (Default=5)	
QPSTATS	Diagnostic printing level for the QP subproblem. **Warning:** Using the ON option can result in very large amounts of output, including the Jacobian.	
	QPSTATS = ON	Turn QP diagnostics on
	QPSTATS = OFF	Turn QP diagnostics off (Default)
QPDEPDIAGS	Flag controlling warning messages on linear dependencies when an active set change causes a singularity	

	QPDEPDIAGS = YES	Messages are written to both OUT file and terminal (Default)
	QPDEPDIAGS = OUT	Messages are written only to OUT file
	QPDEPDIAGS = NO	No messages are written
ACTIVERPT	Flag that controls the reporting of the active set at the end of iteration zero. It is written to the <prob>.out file.	
	ACTIVERPT = YES	Report the active set
	ACTIVERPT = NO	Do not report the active set (Default)
BOUNDRPT.....	Whethwer to report all bounds in the act file	
	BOUNDRPT = YES	Report the bounds (Default)
	BOUNDRPT = NO	Do not report the bounds
IPSIRPT	Flag that controls the reporting of the variables and equations that are the most likely cause of the infeasibility	
	IPSIRPT = NO	Reports no information on the cause of the infeasibility
	IPSIRPT = BRIEF	Reports top 3 variables and equations that are the most likely cause of the infeasibility (Default)
	IPSIRPT = FULL	Reports all variables and equations that are the most likely cause of the infeasibility. **Warning:** Using the FULL option can result in very large amounts of output.
ACTIVESAVE	Whether <prob>.set file is written every time the QP subproblem successfully converges in Opt or Recon cases. This file contains info on which variables were active at bounds. It can be used with "restore active set" param to initialize active set of another run.	
	ACTIVESAVE = YES	Write the file
	ACTIVESAVE = NO	Do not write the file (Default)
ACTIVEINIT	Flag to initialize the active set based on the <prob>.set file as an initial guess of the active set.	
	ACTIVEINIT = YES	Use <prob>.set to initialize the active set
	ACTIVEINIT = NO	Do not use <prob>.set to initialize the active set (Default)
RIGORUPD	Number of constraint updates before a rigorous analysis phase (Default=25)	
QPITER	This parameter indicates the degree of completeness in finding the optimal active set at each QP iteration (for the first 10 iterations). The values are between 1 and 10 with 1 being the most incomplete. **Note:** A number smaller than 10 will increase efficiency but with a potential degradation in robustness. (Default=10)	
QPHESSIANUPD.....	Number of QP Hessian updates kept (Default=20)	
QPCONVTOL.....	Internal QP tolerance. **Warning:** Changing the value from the default may degrade solution performance and robustness. (Default=$1x10^{-10}$)	
USEDROPTOL.....	Whether to drop small nonzeros	
	USEDROPTOL = ON	Drop small nonzeros
	USEDROPTOL = OFF	Do not drop small nonzeros (Default)

DROPTOL ..... Non-zero drop tolerance used to remove small Jacobian values. A larger tolerance will reduce the number of non-zeroes and decrease factorization time. If the value is too large, then the accuracy of the Jacobian will be reduced. This may lead to an increase in the number of iterations and/or singularities. (Default=$1x10^{-20}$)

PIVOTSEARCH..... Maximum number of columns used in pivot search (Default=10)

PIVOTANAL..... Determines Jacobian pivot reanalysis strategy

PIVOTANAL = LOW	Analysis with fill-in monitoring (Default)
PIVOTANAL = MEDIUM	Analysis with no fill-in monitor
PIVOTANAL = HIGH	Analysis at every iteration

ANALTHRESH ..... This parameter controls the automatic reanalysis of the Jacobian by monitoring fill-in. It is invoked once the number of non-zeroes has grown by a factor equal to this parameter. (Default=2)

PIVOTTHRESH..... Pivot selection criterion for improved pivot stability. Values near zero emphasize sparsity and values near one emphasize stability. (Default=0.1)

PIVOTZERO..... Minimum pivot element for near singular problems. If this parameter is set to a positive value, any pivot whose modulus is less than the 'Zero threshold' will be treated as zero. (Default=0.0)

FACTORSPEED..... Linear Matrix factorization method.

FACTORSPEED = NORMAL	Optimizes pivot at every iteration (Default)
FACTORSPEED = FAST	Uses original pivot sequence if possible. This can be faster.

BTF ..... Whether to perform block triangularization

BTF = YES	Perform block triangularization (Default)
BTF = NO	Do not perform block triangularization

MINBTFSIZE ..... Minimum size of a block created during block triangularization (Default=1)

DENSITYRATIO..... Switch from sparse to full matrix processing when the ratio of number of non-zeros in the reduced matrix to the number that it would have as a full matrix is greater than density ratio. (Default=0.7)

SINGULARHAND ..... Strategy for addressing singular problems

SINGULARHAND = NORMAL	Proceed with a passive approach (Default)
SINGULARHAND = ACTIVE	Active set strategy modification (Optimization cases)
SINGULARHAND = STRUCTURAL	Address structural singularities as well
SINGULARHAND = NONE	Abort at any singularity

LUSTATS ..... Diagnostic printing switch for linear algebra

LUSTATS = ON	Print linear algebra diagnostics
LUSTATS = OFF	Do not print linear algebra diagnostics (Default)

FREEONLY..... Whether to include constants (fixed variables) when solving

FREEONLY = YES	Include constants (Default)
FREEONLY = NO	Do not include constants

FACTORSPACE..... Workspace allocated for the solution of the linear system of equations. Problems with excessive fill-in may require a higher number. (Default=6)

ACTIVESPACE ..... Workspace allocated for part of the active set strategy (Default=2)

IWORKF..... Integer work space size multiplier (Default=1)

RWORKF ..... Real work space size multiplier (Default=1)

CWORKF ..... Character work space size multiplier (Default=1)

LSSQP-PARAMS Use to specify parameters for controlling the accuracy, performance, and robustness of the LSSQP solver.

mode ..... Run mode.

mode = DEFAULT	Default for all run modes
mode = SIM	Simulation mode
mode = PARAM	Parameter estimation mode
mode = RECON	Data reconciliation mode
mode = OPTIM	Optimization mode

RELEPS ..... Relative optimization convergence tolerance (RELEPS) used in the Kuhn-Tucker error (KTE) criterion: KTE<=RELEPS * max(0.01, |f|) where f is the objective function value. (Default=$1x10^{-4}$)

RFEASB..... Tolerance on iteration constraint violations. Limit above which feasibility correction will be applied after every iteration. (Default=0.01)

RFINFB ..... Tolerance on final constraint violations. Limit above which feasibility correction will be applied at the end of the optimization calculation. (Default=$1x10^{-6}$)

MAXITER..... Maximum number of SQP iterations allowed (Default=30)

MINITER ..... Minimum number of SQP iterations allowed (Default=2)

MAXLSF..... Maximum number of consecutive SQP iterations with line search failure before terminating LSSQP (Default=10)

MAXQPF..... Maximum number of consecutive SQP iterations with QP failure before terminating LSSQP (Default=10)

NFEASB..... Maximum number of feasibility corrections allowed at each SQP iteration to try to keep constraint violations below the Iterative Constraint Violation Tolerance (Default=2)

NFINFB ..... Maximum number of feasibility corrections allowed to try to reduce constraint violations below the Final Constraint Violation Tolerance after the optimization calculation is terminated (Default=5)

KPTLEV ..... Control panel print level. 1-3 is minimal information, 4 is default information, and 5 is full information. However, other system values are accepted. (Default=4)

KPLLEV ..... Print level for EO solver report file. 1 (Minimal information) through 8 (Full constraint vector) (Default=5)

KPFREQ..... Control the frequency of printing full var/constr. vectors to the EO Solver Report file. The first and last vectors are always printed when requested by the KPLLEV parameter which can be set from the Command Line in the Control Panel. (Default=1)

KPNTOP ..... Control the number of top entries to print in top entry outputs in the EO Solver Report file (Default=10)

MDHESS ..... Hessian approximation option. Generally, this should only be changed for the DRPE case.

MDHESS = 0	Use general BFGS update to approximate the Hessian
MDHESS = 2	Always calculate Gauss-Newton-type Hessian approximation (Default)
MDHESS = 3	Use Gauss-Newton-type Hessian approximation for initialization but update it with BFGS update
MDHESS = 4	Selectively choose between BFGS update or Gauss-Newton-type Hessian approximation

TAUHYB ..... Parameter for deciding whether to use Gauss-Newton-type Hessian approximation for Hessian approximation option=4. (Default=0.1)

LSCOPT ..... Line search options (Default=4)

LSCOPT = 1	Same as option 3 for the first ITRBND iterations, where ITRBND is the parameter for the Number of Bounded Iterations. Perform only step bounding with CHGMAX thereafter, where CHGMAX is the parameter for specifying the Step Size Limit.
LSCOPT = 2	Same as option 4 for the first ITRBND iterations. Perform only step bounding with CHGMAX thereafter.
LSCOPT = 3	Exact penalty function
LSCOPT = 4	Exact penalty function with Powell's Watchdog relaxation (Default)
LSCOPT = 5	Exact penalty function with second-order correction
LSCOPT = 6	Exact penalty function with trust region control
LSCOPT = 7	Exact penalty function with trust region control and second order correction

ITRBND..... Number of initial iterations when the Initial Step Size Limit is used to limit search steps. This parameter, along with the parameter for Initial Step Size Limit, can be used to reduce the step size during the initial iterations. (Default=3)

CHGBND..... Initial limit on the optimization step size (CHGBND). The step size is limited such that ak|dk| <= CHGBND * max(1,|xk|). This is a relative step size limit. A negative value for CHGBND implies an absolute step size limit. (Default=0.25)

CHGMAX..... Step size limit (CHGMAX) after the initial Number of Bounded Iterations. The step size is limited such that ak|dk| <= CHGMAX *max(1,|xk|). (Default=0.5)

BNDAPP ..... Approach to bounds allowed in one iteration. (Default=0.99)

INICHK ..... Iteration count (INICHK) to check if the problem should be reinitialized. LSSQP checks the problem status at the current iteration, INICHK iterations ago and 2*INICHK iterations ago. (Default=20)

LSIZEB1 ..... Whether to resize the Hessian after first iteration

LSIZEB1 = YES	Resize the Hessian (Default)
LSIZEB1 = NO	Do not resize the Hessian

LSIZEB2 ..... Hessian sizing option to specify whether identity matrix or initial Hessian scaling factor is used to set initial Hessian.

LSIZEB2 = SCALED	Use initial Hessian scaling factor (Default)
LSIZEB2 = IDENTITY	Use identity matrix

FSCALF..... Initial Hessian scaling factor, FSCALF. If positive, initial Hessian set to FSCALF*I, else set to |FSCALF|*FSCALV*I where FSCALV is estimate of magnitude of objective function. If FSCALF = 0, value of -0.1 is used. (Default=0.01)

ETASKP ..... Range-space to full step ratio above which BFGS update will be skipped (Default=0.95)

RRLOW ..... Low limit of yTs/sTBs to limit the BFGS update (Default=0.2)

RRHIGH ..... High limit of yTs/sTBs to limit the BFGS update (Default=100.0)

BSMALL..... Smallest diagonal in Choleskey decomposition of the projected Hessian (Default=$1x10^{-8}$)

ZPERTF ..... Perturbation factor for projected Hessian calculation (Default=0.0001)

IFDTYP ..... Finite-difference Hessian approximation type. The frequency of this calculation is determined by the Finite difference frequency parameter.

IFDTYP = HES-NON	Projected Hessian, non-multiplier version (Default)
IFDTYP = HES-NON-DROP	Same as HES-NON, but drop bound contribution
IFDTYP = HES-MUL	Projected Hessian, multiplier version
IFDTYP = DIA-NON	Diagonal approximation, non-multiplier version
IFDTYP = DIA-NON-DROP	Same as DIA-NON, but drop bound contribution
IFDTYP = DIA-MUL	Diagonal approximation, multiplier version

IFDITER..... First iteration at which finite differences are used for Hessian approximation (Default=0)

IFDFREQ ..... Finite difference frequency. Finite differences are used at every nth iteration. (Default=0)

DELTLS ..... Actual to predicted merit function reduction ratio below which a line search step will be rejected (Default=0.1)

MAXLSC ..... Maximum number of line search cutbacks allowed per SQP iteration. When this limit is reached, the SQP iteration continues with the final step size. (Default=1)

ALFALS ..... Minimum step cutback ratio per line search iteration (Default=0.25)

IXSCS ..... LSSQP internal variable and constraint scaling options.

IXSCS = 0	No internal variable or equation scaling (in addition to the scaling performed by models and/or executive)
IXSCS = 3	Derive variable scaling from initial x0; derive constraint scaling from Jacobian
IXSCS = 4	No variable scaling; derive constraint scaling from Jacobian (Default)
IXSCS = 5	Derive variable and constraint scaling simultaneously from Jacobian

BIGSCL ..... Big number to limit scaling (Default=$1x10^{10}$)

SMLSCL ..... Small number to limit scaling (Default=$1x10^{-8}$)

KMUDEC ..... Options for adjusting penalty parameters

KMUDEC = 0	Do not allow penalty parameter to be decreased
KMUDEC = 1	Allow penalty parameter to be decrease gradually (Default)
KMUDEC = 2	Use Lagrange multiplier as penalty parameter. This may work better for some problems

VMUINI ..... Initial line search penalty parameter (Default=0.001)

VMUMIN ..... Minimum line search penalty parameter (Default=$1x10^{-8}$)

VMUFAC ..... Penalty parameter multiplier factor from Lagrange multiplier (Default=2.0)

KFOWDG ..... Accumulated line search counts to force a watchdog step. This relaxes the line search criteria and allows the merit function to decrease. (Default=10)

KBKOUT ..... Number of iterations to wait for merit function to improve before backing out of a forced watchdog relaxation. (Default=20)

LEWBAS ..... Type of basis for range-space representation

LEWBAS = ORTHOGONAL	Orthogonal basis (potentially more stable) (Default)
LEWBAS = COORDINATE	Coordinate basis (less overhead especially for problems with large degrees of freedom)

BNDADJ ..... Adjustment to bounds to create a feasible region when a QP subproblem is infeasible (Default=$1x10^{-5}$)

GNPMAX ..... An artificial weighting factor to drive the QP problem to the feasible region. In rare occasions, it has to be increased to avoid a small feasibility index (Default=$1x10^{6}$)

QPINFE ..... A QP infeasible parameter. If +ive, new search direction is determined by minimizing the sum of absolute violations. This can be helpful when trying to find a feasible solution to an initially infeasible optimization problem. (Default=0.0)

SPDROP ..... Matrix elements with absolute value smaller than this drop tolerance are dropped by the sparse linear solver (Default=$1x10^{-15}$)

NCSRCH ..... Maximum number of columns/row to search for pivot (NCSRCH). > 0: search up to NCSRCH columns; < 0: search up to -NCSRCH columns/rows; = 0: unlimited search (Default=5)

SINGT1 ..... Matrix elements with absolute value less than this cutoff value are not allowed to become pivot elements when selecting a basis (Default=$1x10^{-8}$)

SINGT2 ..... Matrix elements with absolute value less than this cutoff value are not allowed to become pivot elements during numerical factorization (Default=$1x10^{-10}$)

TOLBAS ..... Threshold pivot tolerance when selecting a basis (Default=0.1)

TOLANA ..... Threshold pivot tolerance for the rare case of reanalyzing a matrix (Default=0.1)

LCHBAS ..... Whether to allow basis reselection

	LCHBAS = YES	Allow basis reselection (Default)
	LCHBAS = NO	Do not allow basis reselection

NBDBAS ..... Number of bound violations for insensitive dependent variables before basis reselection (Default=10)

BASFLP ..... Growth of the largest sensitivity matrix element to trigger a new basis selection. The parameter to allow basis reselection must be set to Yes. Set this number to a larger value to prevent LSSQP from reselecting the basis. (Default=100.0)

MSMETH..... Matrix scaling method

MSMETH = 0	Scale with MC19AD
MSMETH = 1	Scale with row and then column equilibration (Default)
MSMETH = 2	Scale with column and then row equilibration

MSFREQ ..... Matrix scaling frequency.

MSFREQ = 0	No matrix scaling
MSFREQ = 1	Scale matrix before a basis selection (Default)
MSFREQ = 2	Scale matrix before an analyze call
MSFREQ = 3	Scale matrix before both basis selection and analysis calls

NUMDER ..... Numerical derivative option. Users should use the numerical derivative options provided by the executive. Potential nonzero in the gradient that are actual zeros should be set to small values for options 2 and 4.

NUMDER = 0	No numerical derivative calculation (Default)
NUMDER = 1	Use numerical derivative for Jacobian
NUMDER = 2	Use numerical derivative for Jacobian and gradient
NUMDER = 3	Verify Jacobian at the initial point
NUMDER = 4	Verify Jacobian and gradient at the initial point

DPERTF..... Relative perturbation size for numerical derivative calculation (Default=$1x10^{-6}$)

XPMIN ..... Absolute perturbation size for numerical derivative (Default=0.01)

DERDIF ..... Relative tolerance for reporting derivative errors (Default=0.001)

DERMIN ..... Absolute tolerance for reporting derivative errors (Default=0.01)

LUBNDS ..... Bounds present flag. Determines whether to consider variable bounds when solving in simulation mode.

LUBNDS = YES	Consider variable bounds (Default)
LUBNDS = NO	Do not consider variable bounds

BIGBND ..... Big number to identify fake bounds (–BIGBND, BIGBND). (Default=$1x10^{20}$)

LINCST..... Linear constraint flag. Determines whether equality constraints are linear.

LINCST = YES	Equality constraints are linear
LINCST = NO	Equality constraints are not linear (Default)

NNDCMP ..... Number of equality constraints that should not be used to eliminate variables (Default=0)

SOLVE Paragraph

Input Language for SOLVE

```
SOLVE
PARAM  keyword=value
```

Optional keywords:

METHOD SEPSEQ

```
RUN-MODE keyword=value
```

Optional keywords:

MODE

```
OPT keyword=value
```

Optional keywords:

OPTOBJ

```
REC keyword=value
```

Optional keywords:

RECOBJ

Input Language Description for SOLVE

PARAM Use to specify the sequential modular or equation oriented solution method for a problem or hierarchy block.

METHOD..... Method of solution to the problem or hierarchy level.

METHOD = SM	Use a sequential modular solution path (Default)
METHOD = EO	Use an equation oriented solution path

SEPSEQ..... Force convergence algorithm to sequence all objects within this hierarchy structure together, independent of objects outside this hierarchy structure.

SEPSEQ = YES	Force
SEPSEQ = NO	Do not force (Default)

RUN-MODE Use to specify the equation-oriented run mode.

MODE..... Equation-oriented run mode.

MODE = SIM	Simulation mode (Default)
MODE = PAR	Parameter estimation mode
MODE = REC	Data reconciliation mode
MODE = OPT	Optimization mode

OPT Use to specify the ID of the objective for optimization.

OPTOBJ..... Objective function used for Optimization run mode. In Simulation mode, this Objective is used but with decision variables fixed.

REC Use to specify the ID of the objective for data reconciliation.

RECOBJ..... Objective function used for Reconciliation run mode. In Parameter Estimation mode, this Objective is used but with decision variables fixed.

49 Measurement Blocks

This chapter describes the input language for MEASUREMENT blocks.

Use the MEASUREMENT block to associate model variables with the actual plant measurements. The model variable could be stream or block variables. For each measurement identified by a tag name, measurement block can either:

- Calculate the offset, given the measured value and the accessed model value.
- Calculate and set the model value, given the measured value and the offset.

MEASUREMENT Block

Input Language for MEASUREMENT

```
MEASUREMENT    mblockid
DEFINE    fvar    vartype    keyword=value
PARAM    MODE=value
CONFIGURATION    idx    keyword=value
```

Keywords:

ENABLED TAGNAME DESCRIPTION PLANT PHYSQTY

Optional keywords:

PLANT-UOM

```
CONNECTION    idx    keyword=value
```

Keywords:

SM-MODEL EO-MODEL

Optional keywords:

MODEL-UOM

```
OFFSET    idx    keyword=value
```

Keywords:

VALUE

Optional keywords:

UOM PHYSQTY

```
BLOCK-OPTIONS    keyword=value
```

Keywords:

SIM-LEVEL TERM-LEVEL

Input Language Description for MEASUREMENT

mblockid ..... Measurement block ID

DEFINE

Use to access a flowsheet variable and equivalence it to a FORTRAN variable, which is used in subsequent CONNECTION sentences to represent the accessed model variable. See Chapter 29 for a complete description of the DEFINE sentence.

fvar ..... Name of the FORTRAN variable.

vartype ..... Variable type. You can use any variable type allowed for the define sentence. (See Chapters 29 and 30.)

PARAM

MODE ..... Specify the calculation mode. The possible calculation modes are:

MODE = CALC-MODEL	Calculate and set accessed flowsheet variables (Model variable)
MODE = CALC-OFFSET	Calculate the difference (offset) between the model variable and plant/measured values
MODE = CALC-PLANT	Calculate plant values by summing offset and model values
MODE = PARAM-OFFSET	Calculate plant or offset values. (Measured-parameterized pair. See the *Aspen Plus User Guide* for more information.)

CONFIGURATION

Use to specify and configure a measurement in a MEASUREMENT block.

idx ..... Measurement number

ENABLED..... Specifies whether a given measurement is enabled. Measurement block will process only measurements that are enabled.

ENABLED = YES	Measurement is enabled
ENABLED = NO	Measurement is disabled

TAGNAME..... Tag name for the measuring instrument. A string of up to 12 characters enclosed in quotes. In Equation-Oriented (EO) mode, measurement variable names are constructed from a tag name and a description. To avoid duplicate variable names, tag name must be unique for each measurement.

DESCRIPTION ..... A brief description (up to 80 characters, enclosed in quotes) of the measuring instrument.

PLANT..... Measured plant value.

PHYSYQTY ..... Physical quantity of the variable being measured. A string of up to 16 characters in quotes. The default is the physical quantity of the associated model variable. See Chapter 3 for physical quantities.

PLANT-UOM ..... The unit of measure for plant value. A string of up to 16 characters enclosed in quotes. The default is the IN-UNIT for physical quantity of the model variable. See Chapter 3 for units of measure.

CONNECTION

Use to associate a Sequential Modular (SM) model variable with an Equation-Oriented (EO) model variable. This sentence is required when the Measurement block is running in EO mode.

idx ..... Measurement number

SM-MODEL..... FORTRAN variable name for accessed flowsheet variable, limited to six characters.

EO-MODEL ..... Equation-Oriented model variable which is equivalent to the specified Sequential Modular flowsheet variable. Used in EO mode. A string of up to 32 characters enclosed in quotes.

OFFSET Use to specify the plant value deviation from the model variable for measurements. The OFFSET sentence is required for each specified measurement when the block's mode is CALC-PLANT or PARAM-OFFSET and offset values are non-zero.

idx ..... Measurement number

VALUE ..... Offset value

PHYSQTY ..... Physical quantity of the offset value. A string of up to 16 characters enclosed in quotes. (See Chapter 3.)

UOM ..... Unit of measure of the offset value. A string of up to 16 characters enclosed in quotes. (See Chapter 3.)

BLOCK-OPTIONS Use to override the diagnostic message levels established by the DIAGNOSTICS paragraph. (See Chapter 45.)

50 Utility Blocks

This chapter describes the input language for UTILITY blocks.

Use the UTILITY block to define variable utilities, where it is assumed that there is a large source of the utility available for use. Many unit operation blocks can use these utilities to represent the supply of heating, cooling, or electricity they require.

UTILITY Block

Input Language for UTILITY

```
UTILITY    uid    GENERAL
COST    price-type=value
```

Price types:

PRICE ELEC-PRICE ENERGY-PRICE

```
PARAM    keyword=value
```

Keywords:

UTILITY-TYPE BASIS COOLING-VALU PRES-IN PRES-OUT T-IN T-OUT VFR-IN VFR-OUT DEGSUB-IN DEGSUB-OUT DEGSUP-IN DEGSUP-OUT CALOPT

```
COMPOSITION    compid  fraction  /  compid  fraction  /  ...
```

Input Language Description for UTILITY

uid ..... Utility block ID

Note: In input files from older versions of Aspen Plus, other utility types besides GENERAL may appear after the uid. This input will still work, but these utility types are superseded by the GENERAL utility type described here, with the specific type such as WATER specified in the PARAM sentence using the UTILITY-TYPE keyword.

COST Use to specify the purchase price of the utility. Specify only one of the following types of cost.

PRICE ..... Price specified in units of $/mass, the direct mass cost of the utility. Do not use with PARAM UTILITY-TYPE=ELECTRICITY.

ELEC-PRICE..... Price specified in units of $/electrical energy. Use only with PARAM UTILITY-TYPE=ELECTRICITY.

ENERGY-PRICE ..... Price specified in units of $/energy, the cost per heating or cooling value of the utility. Do not use with PARAM UTILITY-TYPE=ELECTRICITY.

PARAM **UTILITY-TYPE**..... The type of utility. The possible types are:

UTILITY-TYPE = WATER	Cooling water
UTILITY-TYPE = ELECTRICITY	Electricity
UTILITY-TYPE = OIL	Heating oil
UTILITY-TYPE = GAS	Natural gas
UTILITY-TYPE = COAL	Coal
UTILITY-TYPE = REFRIGERANT	Refrigerant
UTILITY-TYPE = STEAM	Steam

	UTILITY-TYPE = GENERAL	Any composition of components defined in the simulation.
BASIS	Basis for composition specification. Use only with UTILITY-TYPE=GENERAL or REFRIGERANT.	
	BASIS = MASS	Composition specified in mass units
	BASIS = MOLE	Composition specified in mole units
	BASIS = STDVOL	Composition specified in standard volume units
CALOPT	Method for determining heating or cooling value of utility. Do not use with UTILITY-TYPE=ELECTRICITY.	
	CALOPT = DUTY	Heating or cooling value is specified.
	CALOPT = FLASH	Heating or cooling value is calculated by Aspen Plus based on inlet and outlet conditions you specify. Specify two conditions from temperature, pressure, and vapor fraction for each of inlet and outlet. Temperature may be specified as temperature, degrees of subcooling, or degrees of superheating.
COOLING-VALU	Heating or cooling value for utility in energy/mass units. Not used for UTILITY-TYPE=ELECTRICITY	
T-IN	Inlet temperature of utility. When CALOPT=FLASH this is used to determine the heating or cooling value of the utility. When CALOPT=DUTY this is only provided to other programs using this utility data, such as Aspen Pinch.	
T-OUT	Outlet temperature of utility. When CALOPT=FLASH this is used to determine the heating or cooling value of the utility. When CALOPT=DUTY this is only provided to other programs using this utility data, such as Aspen Pinch.	
PRES-IN	Inlet pressure of utility.	
PRES-OUT	Outlet pressure of utility.	
VFR-IN	Inlet vapor fraction of utility.	
VFR-OUT	Outlet vapor fraction of utility.	
DEGSUB-IN	Inlet degrees of subcooling of utility.	
DEGSUB-OUT	Outlet degrees of subcooling of utility.	
DEGSUP-IN	Inlet degrees of superheating of utility.	
DEGSUP-OUT	Outlet degrees of superheating of utility.	
COMPOSITION	Use to specify the composition of the utility with PARAM UTILITY-TYPE=GENERAL.	
compid	Component ID.	
fraction	Fraction of this component, in the basis specified by PARAM BASIS.	

Accessing Variables in UTILITY

Many Aspen Plus features enable you to sample or change block variables. Chapter 29 describes how to access variables. The following tables list variable names and other information needed to sample and/or change variables for this block.

Block Input

Sentence	Variables	ID1
COST	PRICE, ELEC-PRICE, ENERGY-PRICE	—
PARAM	COOLING-VALU, PRES-IN, PRES-OUT, T-IN, T-OUT, VFR-IN, VFR-OUT, DEGSUB-IN, DEGSUB-OUT, DEGSUP-IN, DEGSUP-OUT	—
COMPOSITION	FRAC	cid

Block Results

Description	Sentence	Variable
Total amount of the utility required in mass/time (not applicable to ELECTRICITY)	RESULTS	REQUIREMENT
Total cost of the utility in $/time	RESULTS	COST-RATE
Total energy usage in energy/time.	RESULTS	ENERGY-RATE
Electrical power required (only for ELECTRICITY)	RESULTS	ELEC-RATE
Heating or cooling value of the utility	RESULTS	H-C-VALUE
Inlet temperature.	RESULTS	T-INCALC
Outlet temperature.	RESULTS	T-OUTCALC
Inlet pressure.	RESULTS	PRES-INCALC
Outlet pressure.	RESULTS	PRES-OUTCALC
Inlet vapor fraction.	RESULTS	VFR-INCALC
Outlet vapor fraction.	RESULTS	VFR-OUTCALC
Inlet degrees superheated.	RESULTS	DEGSUP-IN-C
Inlet degrees subcooled.	RESULTS	DEGSUB-IN-C
Outlet degrees superheated.	RESULTS	DEGSUP-OUT-C
Outlet degrees subcooled.	RESULTS	DEGSUB-OUT-C

General Information

This section provides Copyright details and lists any other documentation related to this release.

Copyright

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Related Documentation

Title	Content
Aspen Plus Getting Started Building and Running a Process Model	Tutorials covering basic use of Aspen Plus. A prerequisite for the other Getting Started guides
Aspen Plus Getting Started Modeling Processes with Solids	Tutorials covering the Aspen plus features designed to handle solids
Aspen Plus Getting Started Modeling Processes with Electrolytes	Tutorials covering the Aspen plus features designed to handle electrolytes
Aspen Plus Getting Started Using Equation-Oriented Modeling	Tutorials covering the use of equation-oriented models in Aspen Plus
Aspen Plus Getting Started Customizing Unit Operation Models	Tutorials covering the development of custom unit operation models in Aspen Plus
Aspen Plus Getting Started Modeling Petroleum Processes	Tutorials covering the Aspen Plus features designed to handle petroleum
Aspen Plus User Guide	Procedures for using Aspen Plus
Aspen Plus Unit Operation Models Reference Manual	Information related to specific unit operation models in Aspen Plus
Aspen Plus System Management Reference Manual	Information about customizing files provided with Aspen Plus
Aspen Plus Summary File Toolkit Reference Manual	Information about the Summary File Toolkit, a library designed to read Aspen Plus summary files.
Aspen Plus Input Language Guide Reference Manual	Syntax and keyword meanings for the Aspen Plus input language, and accessible variables.
Aspen Plus OOMF Script Language Reference Manual	Syntax and command meanings for the OOMF Script language
APrSystem Physical Property Methods and Models Reference Manual	Information about property methods and property models
APrSystem Physical Property Data Reference Manual	Information about property databanks
Aspen Plus Application Examples	A suite of examples illustrating capabilities of Aspen Plus
Aspen Engineering Suite Installation Manual	Instructions for installing Aspen Plus and other Aspen Engineering Suite products

Technical Support

Online Technical Support Center

AspenTech customers with a valid license and software maintenance agreement can register to access the Online Technical Support Center at:

http://support.aspentech.com

You use the Online Technical Support Center to:

- Access current product documentation.
- Search for technical tips, solutions, and frequently asked questions (FAQs).
- Search for and download application examples.
- Search for and download service packs and product updates.
- Submit and track technical issues.
- Search for and review known limitations.
- Send suggestions.

Registered users can also subscribe to our Technical Support e-Bulletins. These e-Bulletins proactively alert you to important technical support information such as:

- Technical advisories.
- Product updates.
- Service Pack announcements.
- Product release announcements.

Phone and E-mail

Customer support is also available by phone, fax, and e-mail for customers who have a current support contract for their product(s). Toll-free charges are listed where available; otherwise local and international rates apply.

For the most up-to-date phone listings, please see the Online Technical Support Center at:

http://support.aspentech.com

Support Centers	Operating Hours
North America	8:00 – 20:00 Eastern time
South America	9:00 – 17:00 Local time
Europe	8:30 – 18:00 Central European time
Asia and Pacific Region	9:00 – 17:30 Local time