Aspen Engineering Suite 2004.1

Aspen Plus 2004.1

Getting Started Using Equation Oriented Modeling

aspentech
driving process profitability

Who Should Read this Guide

This guide is suitable for Aspen Plus users who want to start using equation-oriented modeling. Users should be familiar with the procedures covered in *Aspen Plus Getting Started Building and Running a Process Model* before starting these examples.

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Introducing Aspen Plus

Equation Oriented Modeling is a different strategy for solving your flowsheet simulations in Aspen Plus. Configuration of the flowsheet works the same way as previous versions of Aspen Plus, but you choose a different solution strategy for your models.

Equation Oriented Modeling is a very effective way of solving certain kinds of problems, such as:

- the simulation of highly heat-integrated or recycled processes;
- process optimization;
- model tuning via parameter estimation and data reconciliation.

The hands-on tutorial session in this manual demonstrate some of the capabilities of Equation Oriented Modeling.

Getting Started Using Equation Oriented Modeling assumes that you have an installed copy of the Aspen Plus and User Interface software. It further assumes that you are already familiar with using the Aspen Plus User Interface to specify and solve a sequential modular simulation.

Why Use Equation Oriented Modeling?

In Aspen Plus, the standard modeling approach is Sequential Modular (SM). The SM strategy solves each block in the flowsheet in sequence, where given its inlet streams, each block computes its outlet streams. When recycles are present, flowsheet iteration is required. Although effective for many types of simulations, the SM strategy can be very time-consuming for certain types of problems.

Equation Oriented (EO) modeling is an alternate strategy for solving flowsheet simulations. Instead of solving each block in sequence, EO gathers all the model equations together and solves them at the same time. For this reason, EO modeling is sometimes called equation-based or simultaneous equation modeling.

The EO strategy can be very effective for the kinds of problems for which SM is weakest, such as:

- highly heat-integrated processes
- highly recycled processes

- processes with many design specifications
- process optimization
- process model tuning through data reconciliation and parameter estimation

Normally, these types of problems are difficult to solve with SM strategy, because they require many successive solutions to the flowsheet and may contain many nested convergence loops.

Although the number of variables and equations can be very large, EO solves the entire flowsheet simultaneously without nested convergence loops and utilizes analytical first order derivatives. As a result, EO strategy can solve much larger problems using the same computational effort.

Overview of Equation Oriented Modeling

Once a process model is constructed in Aspen Plus, Equation Oriented (EO) modeling is available as a solution technique in addition to the usual Sequential Modular (SM) option for running the simulation.

The first steps in setting up a simulation that uses EO modeling are the same as for setting up any simulation:

- Create a process flowsheet using the Aspen Plus Graphical User Interface (GUI).
- Configure the blocks and streams, using the Data Browser.

Equation Oriented Modeling Input

The SM and EO modeling strategies share most of the input for a simulation. However, some additional input may be desired to further specify an EO simulation. Typical examples of EO input include:

- changing the attributes of variables, including their specifications;
- connecting variables together;
- defining objective functions for optimization problems.

The Data Browser provides EO Configuration forms for specifying EO input and displaying results at the overall flowsheet level, at the hierarchy level, and at the block level.

Equation Oriented Initialization and Solution

The Equation Oriented modeling strategy works well when all variables are “near” the solution. EO strategy is not generally suited to solving a simulation without good estimates for all variables. Therefore, before you solve your flowsheet in EO, you must initialize it in SM.

SM initialization does not require completely converging the SM problem. The minimum requirement is that each block be solved once. How tightly the SM flowsheet needs to be solved to ensure a robust EO formulation is problem-dependent.

When using the Sequential Modular (SM) strategy, Aspen Plus normally runs in a single mode of operation[1]:

SM Solution Mode	Description
Simulation	Model inputs and parameters are fixed. This type of problem has no degrees of freedom. The choice of variables that are specified in the input forms determines which variables are fixed. All the other model quantities are calculated.

The Equation Oriented (EO) strategy can operate in four different modes:

EO Solution Mode	Description
Simulation	This mode is a prediction mode and has no degrees of freedom. For given feed conditions and operating parameters, compute the products.
Parameter Estimation	This mode is a model-tuning mode. It also has no degrees of freedom. Inputs and certain outputs are fixed and model parameters are computed. Parameter Estimation requires one measured variable for each estimated parameter.
Reconciliation	This mode is also used for model tuning. Typically, it minimizes a weighted least squares objective function of deviations between model predictions and plant measurements. This mode may have many degrees of freedom
Optimization	This mode usually involves the manipulation of plant operating conditions (setpoints) to maximize profit, and thus, has degrees of freedom. Parameters determined from a model-tuning mode are fixed during this mode.

[1] The SM strategy does have limited capabilities to operate in modes other than simulation. For example, the Data-Fit feature allows parameter estimation and reconciliation. SM also has an optimization feature. However, the SM approach to Parameter Estimation, Reconciliation, and Optimization generally suffers from long execution times, particularly in complex flowsheets. Consequently, relatively few users have used those SM features to their fullest extent.

EO Variables

The fundamental differences among the EO solution modes are in how the variables are treated. For any mode, the status of a variable may be fixed, free, or a degree of freedom (DOF).

Status	Description
Fixed	The solver cannot change the variable value. It is a fixed input. You specify its value.
Free	The solver determines the variable value as a result of the calculations. Any value you enter before the solution begins is used as an initial guess.
Degree of Freedom (DOF)	The solver is free to move the variable to adjust the objective function. Any value you enter before the solution begins is used as an initial guess.

The status of a variable in any of the four EO solution modes is its *variable specification*.

EO Variable Specifications

The variable specification is an *attribute* of the EO variable. It is a one-word description of the variable's status in each mode. The following table summarizes the allowable specifications.

Specification	Simulation	Parameter Estimation	Reconciliation	Optimization
Calculated	Free	Free	Free	Free
Constant	Fixed	Fixed	Fixed	Fixed
Measured	Free	Fixed	Fixed	Free
Parameterized	Fixed	Free	Free	Fixed
Optimized	Fixed	Fixed	Fixed	DOF
Reconciled	Fixed	Fixed	DOF	Fixed
Independent	Fixed	Fixed	DOF	DOF

The Aspen Plus models define default specifications for all variables, so you only need to enter specifications for the variables you want to change.

In general, the default Aspen Plus specifications indicate that the variable is either:

Fixed in all four modes (specification = Constant)

- *or* -

Free in all four modes (specification = Calculated)

The specifications in the input forms determine which variables are initially Constant.

For example, if the distillate mass flow and reflux ratio are specified in a RadFrac block in SM, then these two variables will have specifications of Constant in EO.

Specifications cannot be set arbitrarily since, for a well-defined EO problem, the net specification of the problem must remain at zero.

Net Specification

The net specification of a problem is defined as:

NSPEC = NVAR – NEQN – NFIX – NDOF

Where:

NSPEC	is the net specification
NVAR	is the number of variables
NEQN	is the number of equations
NFIX	is the number of fixed variables
NDOF	is the number of degree-of-freedom variables

- If the net specification is zero and there are no degree-of-freedom variables, then the problem is *square* and solution can be attempted by nonlinear equation solvers. If there are degree-of-freedom variables, they may be used to minimize or maximize an objective function.
- If the net specification is greater than zero, then the problem is *underspecified* and has many solutions.
- If the net specification is less than zero, then the problem is *overspecified* and there may be no solution.

When Aspen Plus initializes EO from an SM simulation, the problem from SM is square and all the variable specifications are either Constant or Calculated. The variables that are Constant are determined by the quantities specified in the input forms.

If an attempt is made to solve an EO simulation that is underspecified or overspecified, Aspen Plus issues an error message to the Control Panel, and does not attempt to solve the simulation. Since EO simulations are square when they are initialized from SM, the underspecification or overspecification must have been caused by user changes to variable specifications.

In both SM and EO, it is often desirable to change which variables are Constant and which are Calculated. In SM, this is often done using a Design-Spec. However, adding a Design-Spec generally introduces an additional convergence loop to the SM simulation.

In EO, the variable specifications can be changed directly on the EO input forms. This is often done through Spec Groups. Aspen Plus requires that the net specification remains unchanged within a Spec Group for all solution modes to ensure that the problem remains well defined.

For Parameter Estimation and Reconciliation modes, you may want to Fix different variables than in Simulation and Optimization modes. Use the Measured and Parameterized variable specifications to indicate such relationships.

Degrees of freedom for Optimization and Reconciliation runs may be created by making a Constant variable Reconciled, Optimized, or Independent. These specifications will create degrees of freedom in the Reconciliation or Optimization modes. The Simulation and Parameter Estimation modes are square.

Other EO Variable Attributes

In addition to the specification, variables have other attributes that may be set through the EO input forms. They include:

Attribute	Description
Value	The initial value of the variable. If the variable is free during solution in the selected mode, the solution engine may change the value.
Lower Bound [2]	The minimum allowable value of the variable.
Upper Bound [2]	The maximum allowable value of the variable.
Step Bound [2]	A change limit on the variable. This represents the maximum amount by which a variable may change between the beginning and end of a solution. The solution engine uses the most restrictive of the Lower, Upper, and Step bounds.
UOM	The units of measure of the variable. The default UOM is the output units selected for the Aspen simulation. This may be changed to any valid Aspen Plus unit, based on the physical type of the variable.
Bound Type	One of the following: Hard indicates that the bound will be respected at all times. This is the default. Relaxed indicates that if the bound is violated at the start of the solution, it may be relaxed, that is, moved to the current variable value. Soft indicates that any violation of the bound is multiplied by the soft bound weight and added to the objective function (penalty function).
Soft Bound Weight	Weighting factor used when the Bound Type is Soft.

Limitations of EO in Aspen Plus 2004.1

Aspen Plus is not able to solve all SM problems with the EO approach. Certain features that have been implemented for SM have not been implemented in EO. Refer to *What's New in AES 2004.1* for a detailed list of which SM features are not supported by EO.

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2 Although the upper and lower bounds may be specified for all variables, they are not always enforced. Whether or not the bounds are enforced (and if so, how they are enforced) depends on the mode and choice of convergence algorithm. A detailed discussion of the EO convergence algorithms and their treatment of bounds in the various modes is beyond the scope of this manual. For more information, refer to the *Aspen Plus User Guide*.

If an EO simulation includes unit operation models that are not supported by EO, EO will employ the *perturbation layer* to solve that portion of the simulation. The perturbation layer isolates the unsupported block and obtains derivatives for the unsupported block by numerical perturbation. While this does allow certain unsupported models to be included in an EO simulation, it can greatly increase execution time, and is not generally recommended.

A detailed discussion of the perturbation layer is beyond the scope of this manual. For details on the perturbation layer, refer to the *Aspen Plus User Guide*.

Sessions in this Book

Getting Started Using Equation Oriented Modeling provides five sessions, which illustrate the following concepts:

- EO Solution Modes

  Simulation

  Parameter Estimation

  Reconciliation

  Optimization
- Variable Specifications

  Controlling how variables are treated in each mode
- Connections

  Defining connections

  How connections work
- Model Tuning

  The Measurement model

  Parameter Estimation

  Reconciliation
- Optimization

  Defining an objective function
- Mixing SM and EO in one simulation

  EO treatment of Calculators, Design-Specs and Sensitivity

  Solving a flowsheet in Mixed Mode

Follow the steps in this chapter	To learn how to
1 Basic Operations	Run a problem in EO. Change variable specifications and other attributes. Define a linear objective function. Solve an economic optimization problem.
2 Heat Integration	Use the HXFlux model. Define a reduced set of Model Components. Define connections.
3 Parameter Estimation	Use Parameter Estimation to tune the models to process data. Use the Measurement model.
4 Reconciliation	Use Reconciliation to tune the models to process data. Define a sum of squares objective function.

Using Backup Files

Because each chapter assumes familiarity with the preceding ones, we recommend that you perform the sessions *sequentially*.

Aspen Plus provides backup files containing all problem specifications and results for each tutorial session. You can use the backup files to check your results.

1 Basic Operations

This session demonstrates the basic functionality of Aspen Plus Equation Oriented (EO) modeling, including an economic optimization.

You will:

- Set up a RadFrac distillation column model and run a standard (Sequential Modular or SM) simulation.
- Use EO modeling to quickly and easily specify desired product stream characteristics and determine the operating conditions needed to meet your specifications.
- Perform an economic optimization to obtain the maximum profitability while product stream characteristics remain in a specified range.

The tutorial sessions in this Getting Started Guide assume that you have completed all of the sessions in *Getting Started Building and Running a Process Model*. In particular you should be able to:

- Start Aspen Plus (using a blank simulation, template, or existing simulation).
- Place blocks and streams.
- Navigate from form to form using the Data Browser menu tree.
- Enter data into the required fields in the input sheets.
- Run a simulation
- View the data in the results sheets.
- Save a simulation.

Allow about 45 minutes for this session.

Defining the Simulation

Construct a distillation model for separating an ethane/ethylene feed stream. The simulation that you will construct is shown in Figure 1.1. There is one feed stream, one unit operation block, two product material streams, and one outlet heat stream.

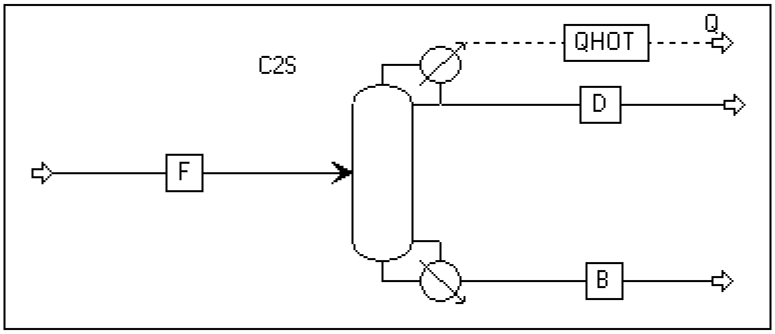


Figure 1.1 Ethylene Distillation

Given the feed stream component mole fractions and total flow rate, the distillate flow rate, reflux ratio, and Murphree efficiencies for the distillation column, Aspen Plus will calculate the component mole fractions in the product streams.

After running the simulation in Sequential Modular (SM) mode, you will use the Equation Oriented modeling capabilities of Aspen Plus to directly control which variables are specified as input and which are calculated. In this example, you will specify the component mole fractions in the product streams and Aspen Plus will calculate the required distillate flow rate and reflux ratio.

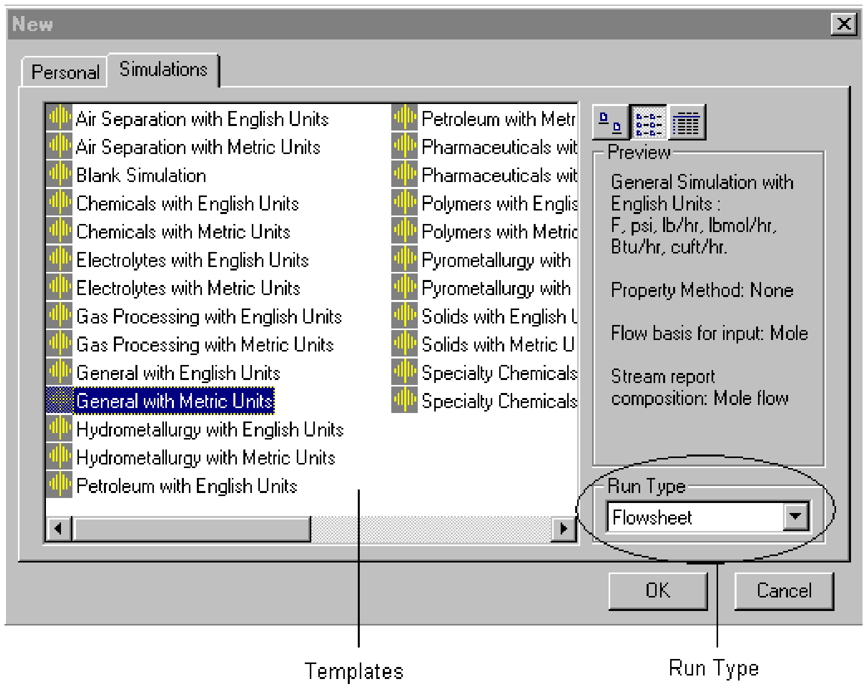
Setting Up the SM Simulation

First set up a simulation for an ordinary SM run. As usual, you will open a new simulation, build a process flowsheet, specify global simulation characteristics such as title and property method, and specify stream and block characteristics.

Open a New Simulation

1 Start Aspen Plus, then select **Template** in the **Aspen Plus Startup** dialog box and click **OK**.

2 In the **New** dialog box, select the **General with Metric Units** template, select the **Flowsheet** Run Type, and click **OK**.



The **Aspen Plus** window is now active.

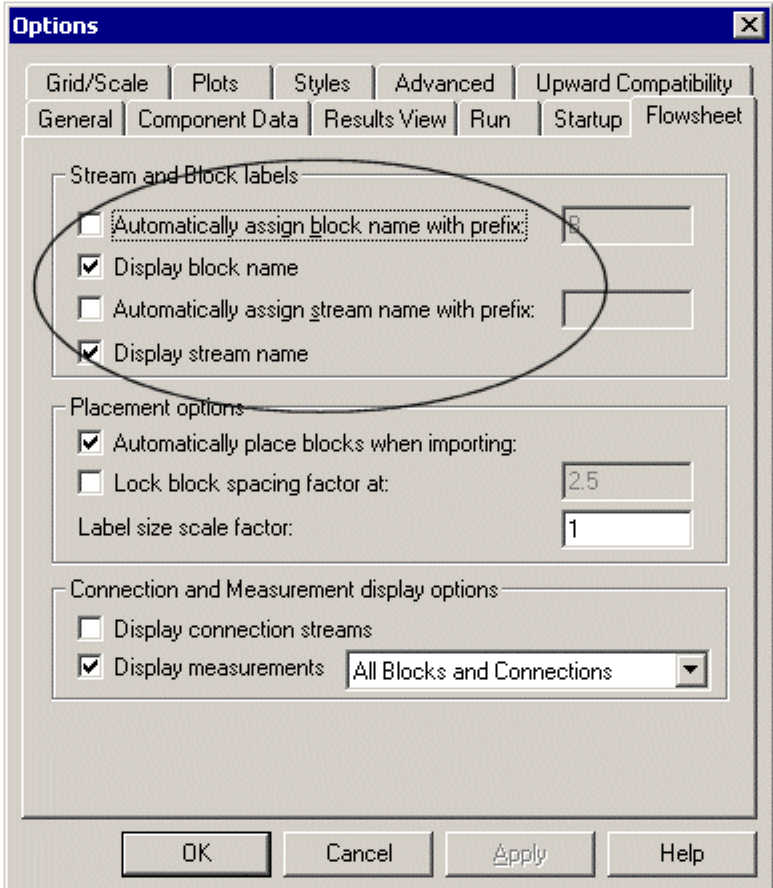
3 From the **Aspen Plus** menu bar, choose **Tools | Options**.

The **Options** dialog box appears.

4 In the **Options** dialog box, click the **Flowsheet** tab.

5 Clear the **Automatically assign block name with prefix** checkbox.

6 Clear the **Automatically assign stream name with prefix** checkbox.



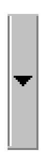
7 Click **OK**.

8 Save the simulation file as **EO1apw**.

For the distillation column, use the RadFrac FRACT1 icon and name the block **C2S**. Create a feed stream (**F**), a liquid distillate stream (**D**), a bottoms stream (**B**), and a condenser heat stream (**QHOT**) and connect them to the block.

Build the Process Flowsheet

1 In the **Model Library**, click the **Columns** tab to display the available distillation columns.

2 Click the arrow  next to the RadFrac model, select the **FRACT1** icon, and drop it on the flowsheet.

The **Input** dialog box appears.

3 Name the block **C2S** and click **OK**.

4 On the flowsheet, connect the following streams to the RadFrac column:

Stream ID	Stream Type	Port
F	Material	Feed (required)
D	Material	Liquid Distillate (required if distillate vapor fraction < 1)
B	Material	Bottoms (required)
QHOT	Heat	Condenser Heat Stream (optional)

5 Click the **C2S** label and drag it (holding the mouse button) to any desired location. For example, you can place it inside the block icon.

Your Process Flowsheet should now look like Figure 1.1.

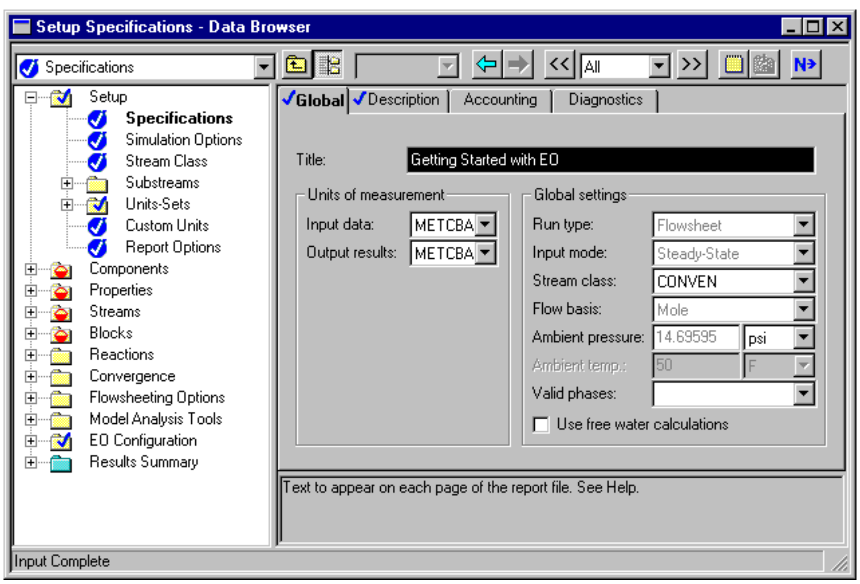
The next step is to specify a title, components used in the simulation, the property method to be used for calculations, the report options, and the feed stream characteristics.

Enter Title, Components, Base Method, Report Options, and Feed Specs

1 Open the **Data Browser** (click  or press **F8**).

2 Go to the **Setup | Specifications | Global** sheet.

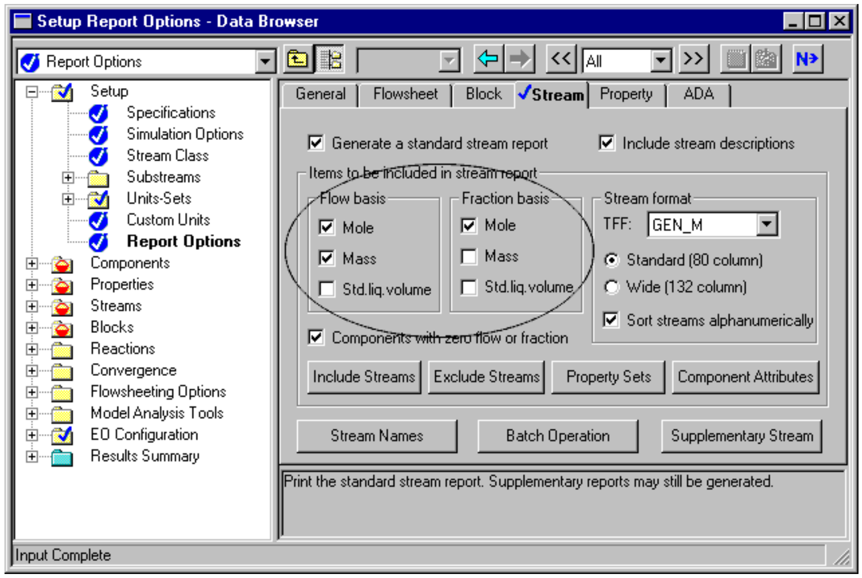
3 Enter a title.



4 Go to the **Setup | Report Options | Stream** sheet.

5 Under Flow basis, note that **Mole** is already selected, and select **Mass** as well.

6 Under Fraction basis, select **Mole**.

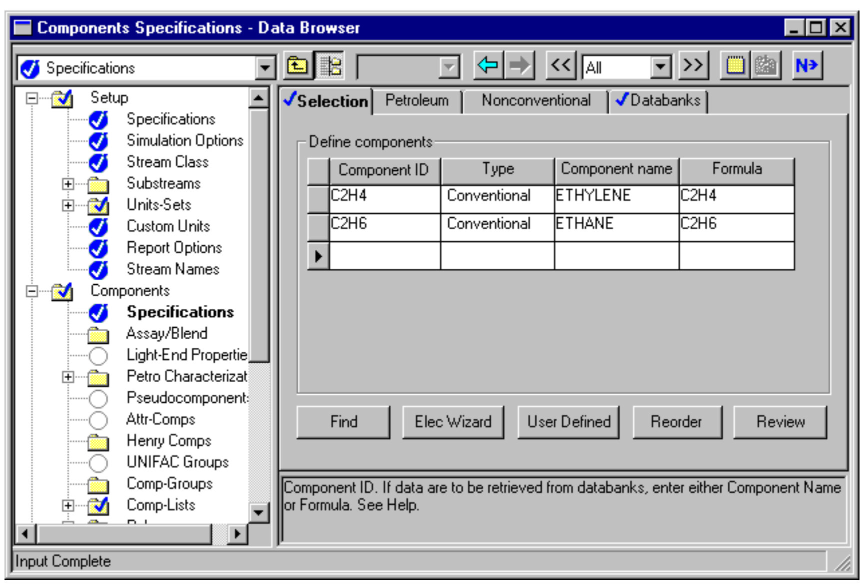


7 Go to the **Components | Specifications | Selection** sheet.

8 Enter the following components:

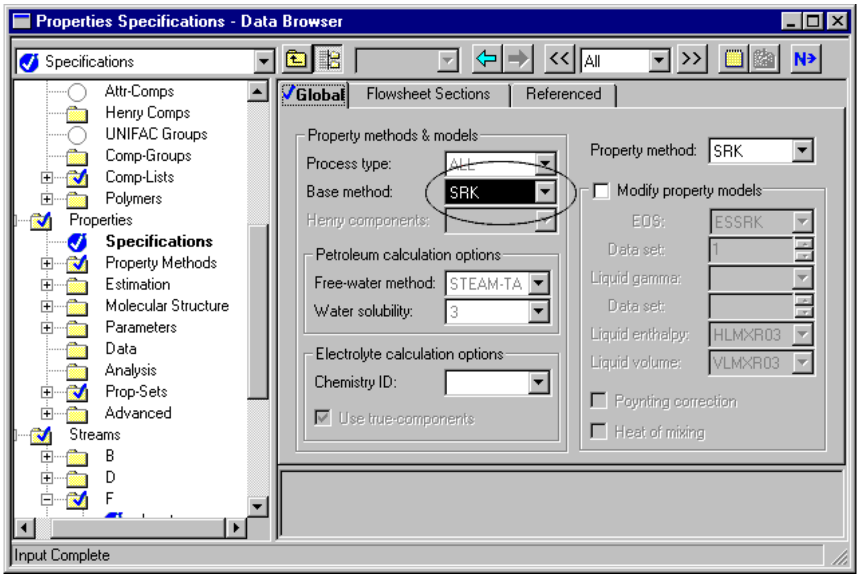
Component ID	Type	Component Name	Formula
C2H4	Conventional	Ethylene	C2H4
C2H6	Conventional	Ethane	C2H6

If you type the Component ID and press **Enter** on the keyboard, Aspen Plus will fill in the three remaining fields since it recognizes the IDs for ethylene and ethane.



9 Go to the **Properties | Specifications | Global** sheet.

10 In the **Base method** field, select SRK.

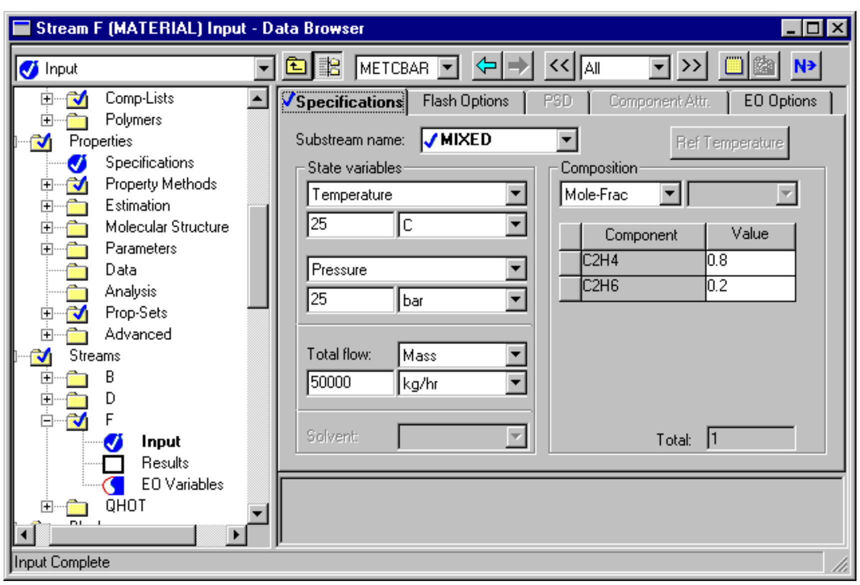


11 Go to the **Streams | F | Input | Specifications** sheet.

12 Enter the following specifications for the feed stream:

Field	Value
Temperature	25 C
Pressure	25 bar
Total Flow	Mass 50000 kg/hr
Composition	Mole-Frac
C2H4 mole fraction	0.8
C2H6 mole fraction	0.2

Choose the **Mass** option for Total flow before selecting **kg/hr** so that these units are available. Choose **Mole-Frac** from the first drop down list in the Composition area.



The last major step in setting up the simulation is to configure the RadFrac distillation column model (**C2S**). Specify the number of stages, the distillate rate and reflux ratio, the entry stage for the feed stream, and a pressure profile for the column. Finally, set the Murphree efficiencies for all stages.

Configure the RadFrac Block

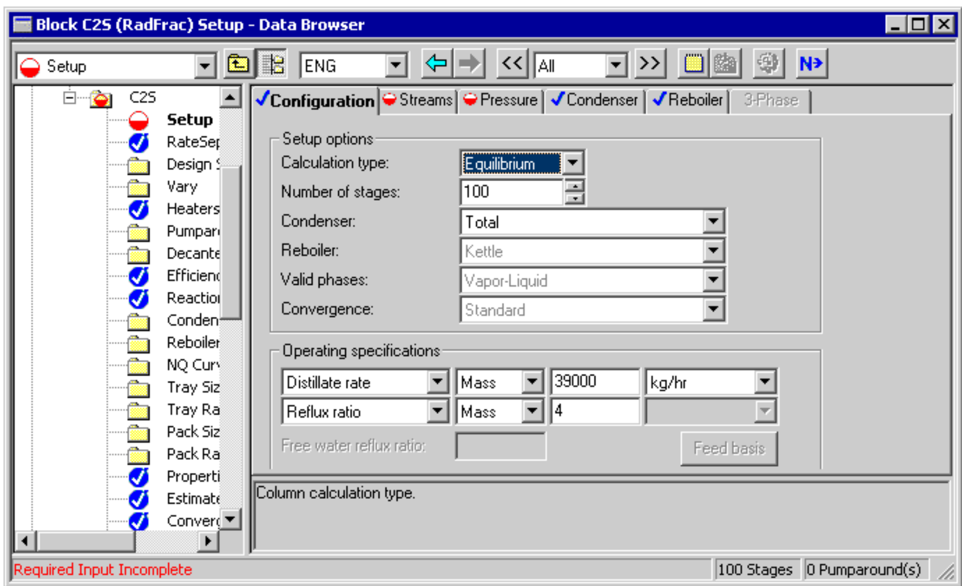
1 On the **Blocks | C2S | Setup | Configuration** sheet, specify the following Setup options:

Field	Value
Number of stages	100
Condenser	Total

2 Specify the following Operating specifications:

Field	Value
Distillate rate	Mass 39000 kg/hr
Reflux ratio	Mass 4.0

For the Distillate rate specification, select **Mass** before selecting the **kg/hr** units.

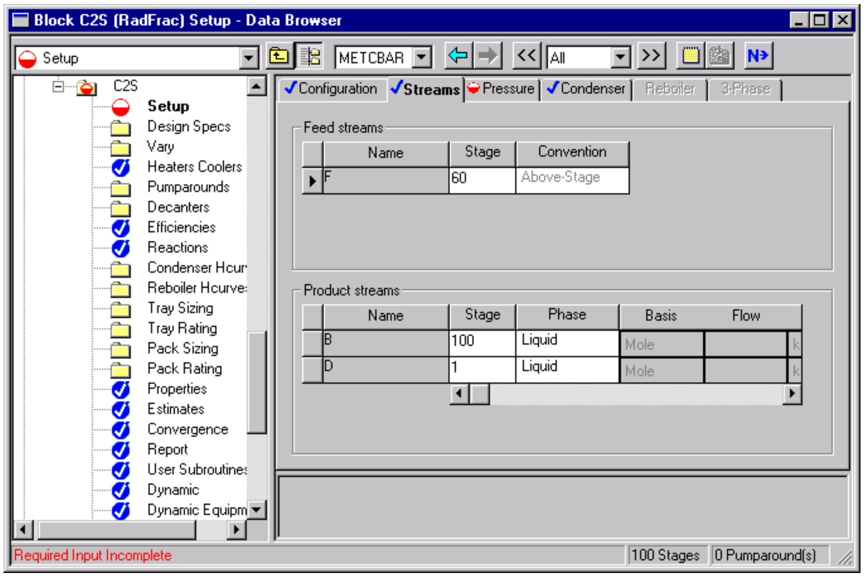


3 Click the **Streams** tab to display the **Blocks | C2S | Setup | Streams** sheet.

4 In the Feed streams area, specify the following values for stream **F**:

Column	Value
Stage	60
Convention	Above-Stage

5 In the Product streams area, verify that the **Phase** for both product streams is **Liquid**.

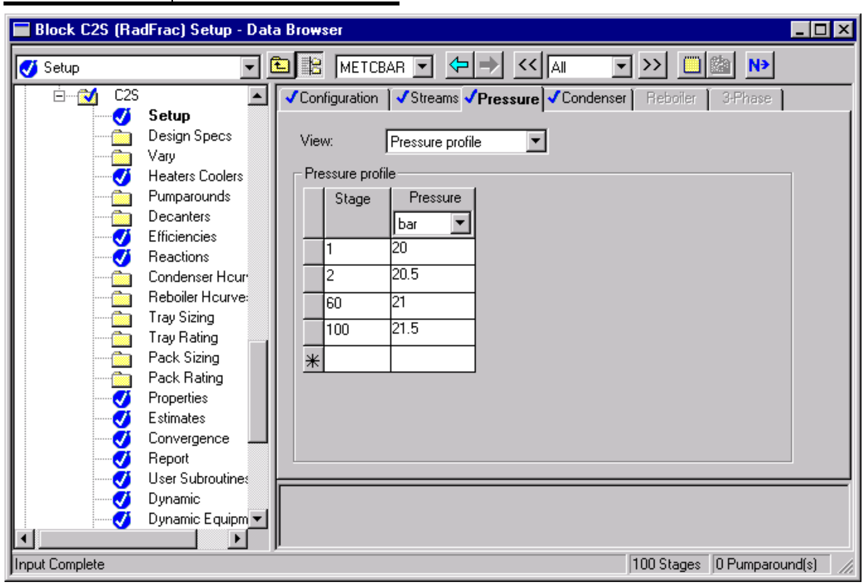


6 Click the **Pressure** tab to display the **Blocks | C2S | Setup | Pressure** sheet.

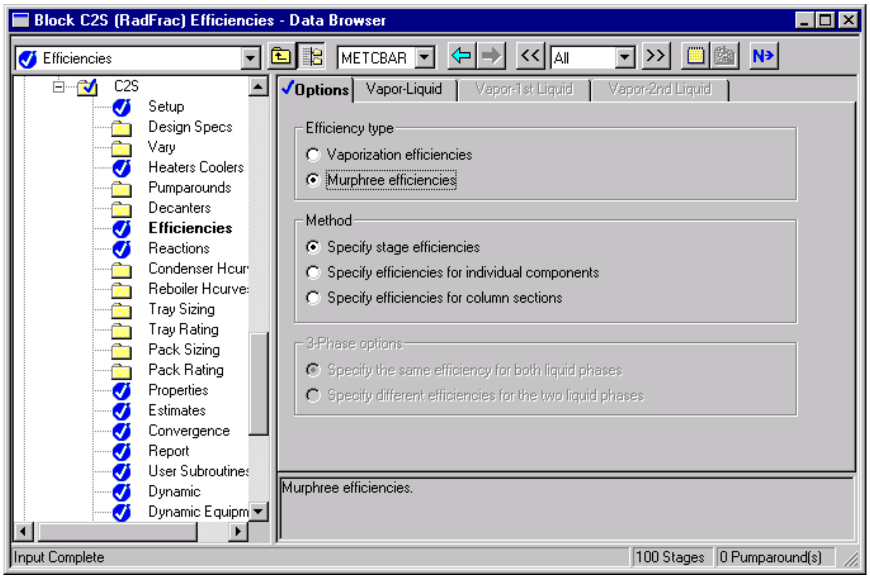
7 In the **View** field, select **Pressure profile**.

8 Enter these stage pressures in **bar** units:

Stage	Pressure
1	20
2	20.5
60	21.0
100	21.5



9 Go to the **Blocks | C2S | Efficiencies | Options** sheet and select the **Murphree efficiencies** in the Efficiency type area.

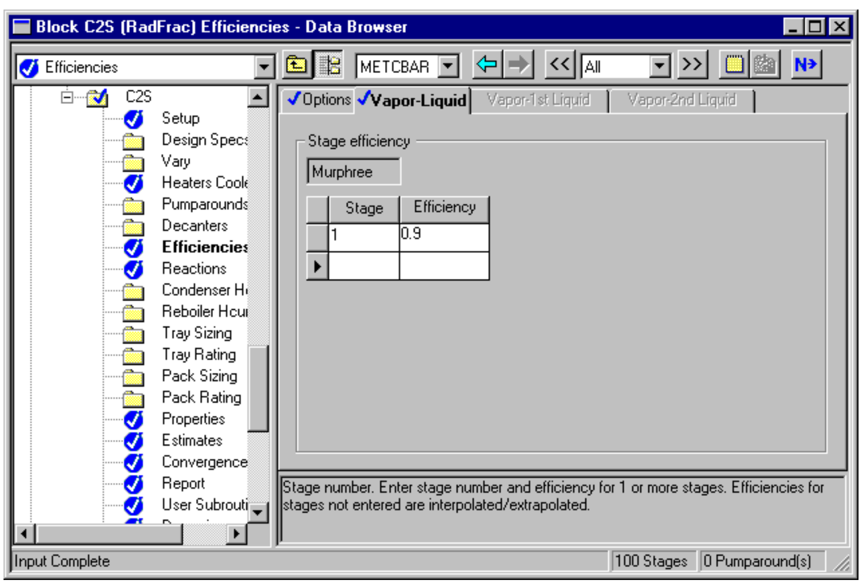


10 Click the **Vapor-Liquid** tab to display the **Blocks** | **C2S** | **Efficiencies** | **Vapor-Liquid** sheet.

11 Enter these stage and efficiency values:

Stage	Efficiency
1	0.9

This causes an efficiency of 0.9 to be used for all stages.

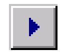


You have completed the specifications and are now ready to run the simulation.

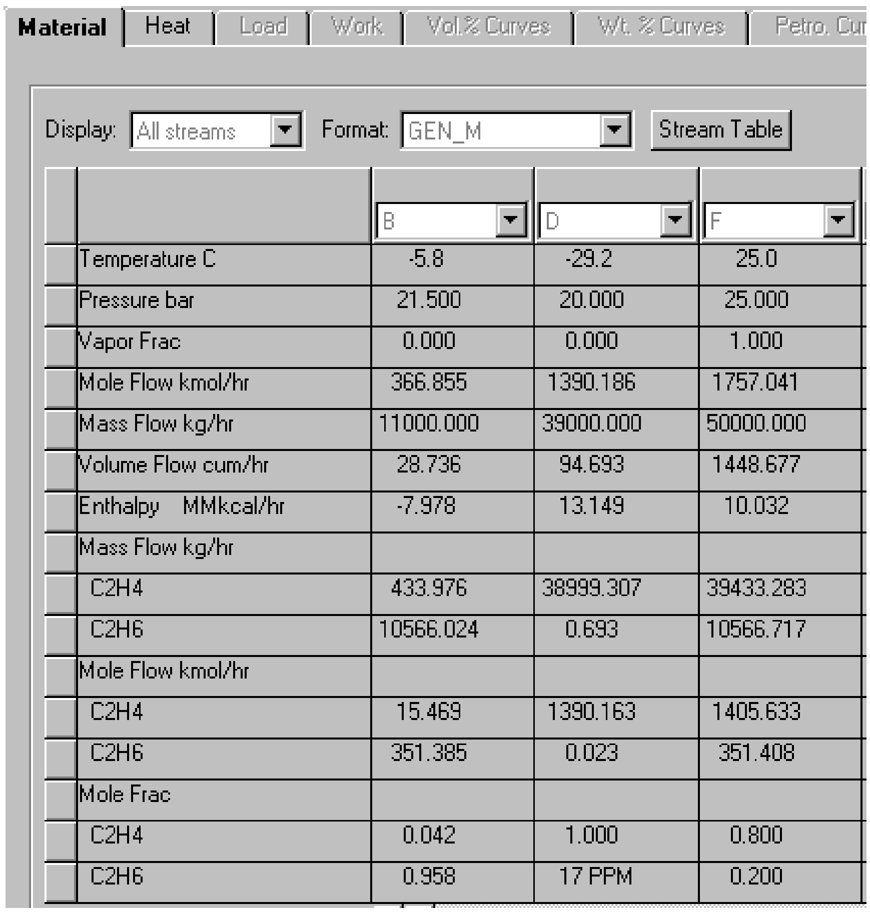
12 Save the simulation file so that your work is safe.

Running the Simulation and Examining the Results

1 From the Aspen Plus menu bar, choose **View | Control Panel**.

2 On the **Control Panel** toolbar, click  to run the simulation.

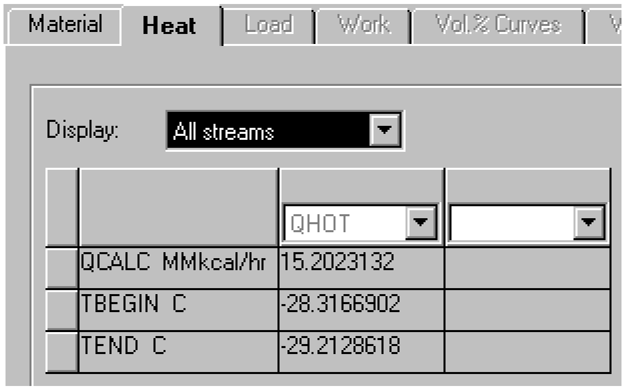
3 When the simulation calculations are completed, go to the **Results Summary | Streams | Material** sheet and note the purity of the distillate and bottoms streams.



	B	D	F
Temperature C	-5.8	-29.2	25.0
Pressure bar	21.500	20.000	25.000
Vapor Frac	0.000	0.000	1.000
Mole Flow kmol/hr	366.855	1390.186	1757.041
Mass Flow kg/hr	11000.000	39000.000	50000.000
Volume Flow cum/hr	28.736	94.693	1448.677
Enthalpy MMkcal/hr	-7.978	13.149	10.032
Mass Flow kg/hr			
C2H4	433.976	38999.307	39433.283
C2H6	10566.024	0.693	10566.717
Mole Flow kmol/hr			
C2H4	15.469	1390.163	1405.633
C2H6	351.385	0.023	351.408
Mole Frac			
C2H4	0.042	1.000	0.800
C2H6	0.958	17 PPM	0.200

The distillate stream is almost 100% ethylene (C2H4) and the bottoms stream is 95.8% ethane (C2H6). This was achieved with a distillate rate of 39,000 kg/hr and a reflux ratio of 4.0.

4 Click the **Heat** tab to display the **Results Summary | Streams | Heat** sheet.



The condenser at the top of the column required about 15.2 MMkcal/hr of cooling in order to achieve the specified distillate rate and reflux ratio. Aspen Plus also reports the temperatures over which this duty was expended.

In the next sections, you will use EO modeling to specify product purities and perform an economic optimization.

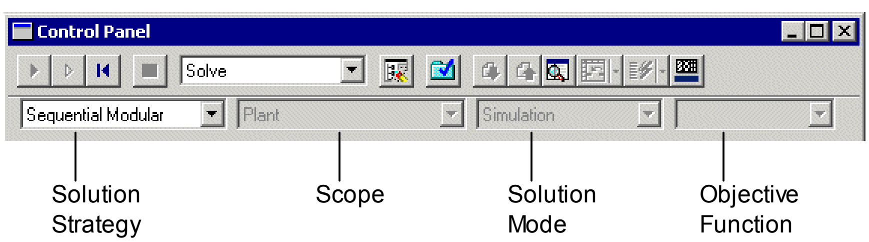
Running an EO Simulation

You have completed a Sequential Modular (SM) simulation so all variables are initialized. Now you can change the solution strategy to Equation Oriented (EO).

Solve the Problem Using EO

1. Go to the **Control Panel**.
2. Click More at the bottom of the Control Panel window to display the EO controls.

   Additional run options appear below the tool bar, as shown:

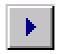
   

3. From the **Solution Strategy** list, select **Equation Oriented**.

   Changing the strategy to EO:

   – Activates the Scope, Mode and Objective Function fields.
   – Builds the EO flowsheet and initializes the EO variable values from the SM solution. This is called *synchronization*.

   Control Panel messages indicate that all SM blocks were successfully placed on the EO flowsheet.

4 Click  to run the simulation in the Equation Oriented (EO) solution strategy.

```
<reset scope>
<solver DMO>
<set mode = sim>
<apply solver settings>
<solve none>


            Residual   Objective   Objective    Overall       Model
          Convergence Convergence  Function  Nonlinearity Nonlinearity  Worst
Iteration   Function    Function     Value       Ratio        Ratio     Model
--------- ----------- ----------- ---------- ------------ ------------ --------
     0      2.621D-06   0.000D+00  0.000D+00    1.000D+00    1.000D+00 C2S
     1      4.597D-14   0.000D+00  0.000D+00

Successful solution.


Optimization Timing Statistics         Time      Percent
================================      ========   =======

MODEL computations                     0.32 secs    64.00 %
DMO computations                       0.06 secs    12.00 %
Miscellaneous                          0.12 secs    24.00 %
--------------------------------      ---------    -------
Total Optimization Time                0.50 secs   100.00 %

Problem converged
```

The Control Panel reports the following information:

– The Solver used - DMO
– The solution mode - Simulation
– Diagnostics for every iteration of the solver

Notice that Iteration 0 reflects the convergence status at the end of EO initialization from SM.

The information reported for each iteration includes:

– Residual Convergence Function

This is a measure how close the equations are to being solved. After one iteration, the Residual Convergence Function is less than 1.E-6, so the problem is converged. Since the EO simulation is solving the same problem as the SM simulation, EO solves the problem in one iteration after being initialized from the SM solution at synchronization time

– Objective Convergence Function and
Objective Function Value

This information is only relevant for EO Optimization and Reconciliation solution modes.

– Overall Nonlinearity Ratio

This is a measure of the nonlinearity of the overall problem. The closer the Nonlinearity Ratio is to 1.0, the more linear the problem. A negative value indicates that the problem behaves in the opposite of what is expected. Near the solution, as step sizes decrease, this value should approach 1.0.

– Model Nonlinearity Ratio

This is the Nonlinearity Ratio for the worst model.

– Worst Model

This is the model whose nonlinearity is furthest in absolute value from 1.0.

Finally, the Control Panel displays statistics regarding how much time was required by the various modules of the program to solve the problem.

Identifying EO Variables

Every equation-oriented (EO) model generates variables and equations with names containing the names of their corresponding blocks, streams, and components. The format is:

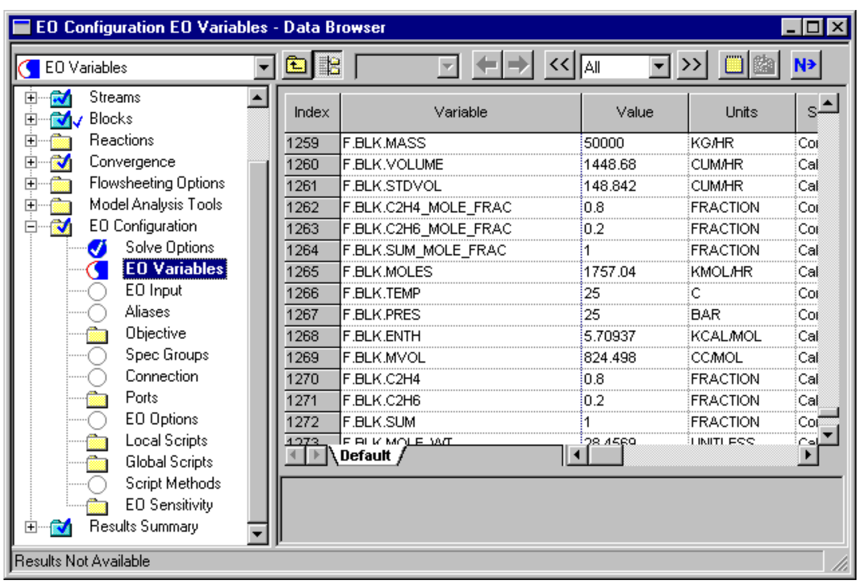
blockid.variableid.description

Where:

blockid	Is the block name, including hierarchy names, if appropriate.
variableid	Is normally **BLK**, indicating a variable within the block, or ***streamid*.STR**, indicating an inlet or outlet stream of the block.
description	Is a short description of the variable.

For example, the first variable on the EO variable grid, **C2S.F.STR.MOLES**, refers to the total molar flow rate (MOLES) of stream F (F.STR) which goes in or out of block C2S (C2S).

The **EO Configuration | EO Variables** form in the Data Browser (shown below) lists every EO variable and displays information such as Value, Units, and Specification about each one.



Note that variables beginning with F.BLK correspond to an EO block that represents the flowsheet feed stream. The creation of this block (there is only one in this case since there is only one feed stream) enables the user to set up an EO simulation in which the feed conditions to the flowsheet vary during the calculation.

Specifying Product Purities

Next, you will change the specifications of the EO variables so that the distillate ethane and bottoms ethylene mole fractions are fixed and the distillate mass flow rate and the reflux ratio are calculated.

In an SM simulation, you would use the **Design Specs** and **Vary** object managers that appear beneath the **C2S** block in the Data Browser menu tree or you would use external Design Specs. In an EO simulation, you can simply change the variable specifications from Calculated to Constant or from Constant to Calculated.

You can temporarily change variable specifications on the **EO Configuration | EO Variables** form. This form is a long list of every variable in the simulation and is cumbersome to use. Also, any changes made here are not saved, and there is no error checking to avoid creating an improperly specified problem.

The **EO Configuration | Spec Groups** form provides a permanent and convenient way to change variable specifications. Use this form to create a Spec Group – a list of variables with their specifications that may be enabled or as needed. Multiple Spec Groups can be specified for each simulation and enabled or disabled depending on the Solution Mode being used.

After you create a Spec Group and reinitialize or run the simulation, the new specifications appear on the **EO Configuration EO Variables** form.

Note: A Spec Group must not change the net specification of the problem. A Spec Group that would change the net specification is not processed, and appears with a status of Inactive on the **Spec Groups** form.

Spec Groups forms are located at three different levels in the Data Browser menu tree:

- Within individual block folders
- The hierarchy-level EO Configuration folder
- The top-level EO Configuration folder

You will implement a Spec Group in the top level EO configuration folder. The Spec Group will list variables and specifications for the distillate mass flow, the reflux ratio, and for ethylene and ethane concentrations in the two product streams.

Define a Spec Group

1 Go to the **EO Configuration | Spec Groups** form to open the Spec Groups Object Manager.

2 In the first **Spec group** field, enter **C2COMPS** and press **Enter** on the keyboard.

3 Select the **C2COMPS** row and click **Edit**.

   The **Define Spec Groups** dialog box appears.

4 In the **Description** field, enter *Fix the tower compositions*.

5 Enter the following variable names and user specs:

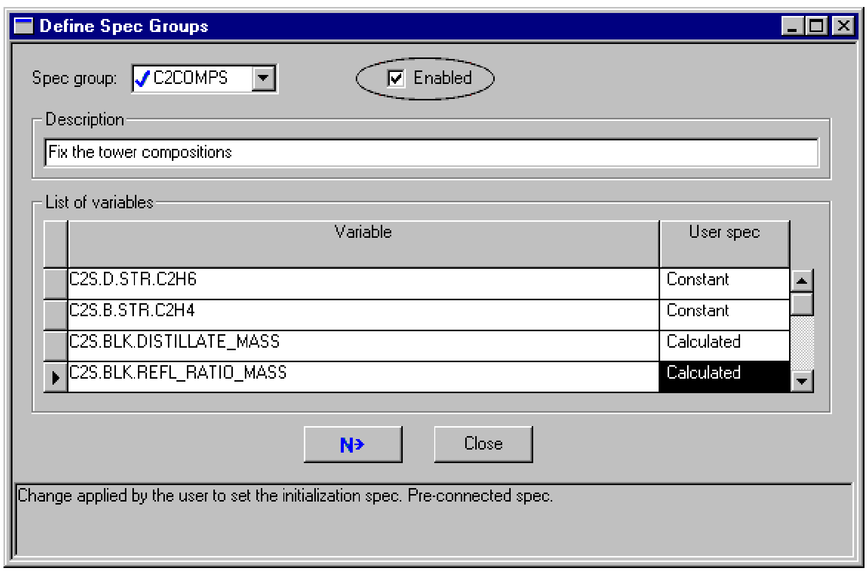
Variable	User Spec
C2S.D.STR.C2H6	Constant
C2S.B.STR.C2H4	Constant
C2S.BLK.DISTILLATE_MASS	Calculated
C2S.BLK.REFL_RATIO_MASS	Calculated

Tip: You can type the variable names, copy and paste variable names from the EO Variables form, or place the cursor in the **Variable** field and click the button that appears at the end of the field to open the EO Variables "Finder" dialog box.

The distillate mass flow and mass reflux ratio were both previously Constant while the distillate and bottoms ethane and ethylene concentrations were previously Calculated. Therefore, this Spec Group does not change the net specification of this problem.

6 Verify that the **Enabled** checkbox is selected.

The **Define Spec Groups** for C2COMPS is complete:



7 Click **Close** to close the dialog box.

8 Press **Shift-F5** or click , then click **OK** to reinitialize the EO simulation with the new variable specifications.

9 Go to the **EO Configuration | EO Variables** form.

10 Double-click the **Specifications** column header to list all Calculated variables first. Double-click a second time to list all Constant variables first.

Tip: You can double-click any of the column headers on this form to sort variables by that column. For example if you double-click the **Variable** header, variables will sort alphabetically by name; double-click again to sort in reverse alphabetical order.

Index	Variable	Value	Units	Specification
14	C2S.D.STR.C2H6	1.65875e-005	FRACTION	Constant
20	C2S.B.STR.C2H4	0.0421219	FRACTION	Constant
41	C2S.BLK.EFF_1	0.9	UNITLESS	Constant
1251	C2S.BLK.PSPEC_1	20	BAR	Constant
1252	C2S.BLK.PSPEC_2	20.5	BAR	Constant
1253	C2S.BLK.PSPEC_60	21	BAR	Constant
1254	C2S.BLK.PSPEC_100	21.5	BAR	Constant
1259	F.BLK.MASS	50000	KG/HR	Constant
1262	F.BLK.C2H4_MOLE_FRAC	0.8	FRACTION	Constant
1263	F.BLK.C2H6_MOLE_FRAC	0.2	FRACTION	Constant
1266	F.BLK.TEMP	25	C	Constant
1267	F.BLK.PRES	25	BAR	Constant
1272	F.BLK.SUM	1	FRACTION	Constant

The two variables you specified as Constant in the Spec Group appear along with the variables you specified on the input sheets for the SM simulation. The two product stream concentrations are now Fixed quantities; their values are taken from the results of the SM run you performed previously.

11 Scroll toward the bottom of the EO variables list to examine the distillate and bottoms flow variables.

Index	Variable	Value	Units	Specification
1233	C2S.BLK.DISTILLATE_MOLE	1390.2	KMOL/HR	Calculated
1234	C2S.BLK.DISTILLATE_MASS	39000.5	KG/HR	Calculated
1235	C2S.BLK.DISTILLATE_STDV	117.766	CUM/HR	Calculated
1236	C2S.BLK.BOTTOMS_MOLE	366.837	KMOL/HR	Calculated
1237	C2S.BLK.BOTTOMS_MASS	10999.5	KG/HR	Calculated
1238	C2S.BLK.BOTTOMS_STDV	31.0753	CUM/HR	Calculated
1239	C2S.BLK.REFL_RATIO_MOLE	3.99995	UNITLESS	Calculated
1240	C2S.BLK.REFL_RATIO_MASS	3.99995	UNITLESS	Calculated
1241	C2S.BLK.REFL_RATIO_STDV	3.99995	UNITLESS	Calculated

The distillate flow rate and reflux ratio are now treated as Free quantities.

Running an EO simulation now would have no effect since the previous solution is still valid. However, you will now change the values of the two product stream concentrations and run the simulation. This will cause the distillate flow rate and reflux ratio to change.

Enter Values for the Product Stream Concentrations

1 Go to the **EO Configuration | EO Input | Configure** sheet.

2 Click in the **Variable or alias** field and click .

The **EO Variables** dialog box appears displaying the complete list of EO variables.

3 Click to display the attributes for each variable.

4 Click the **Specification** column header once.

This sorts all variables by their current variable specification in alphabetical order. All Calculated variables appear first, followed by all Constant variables.

5 Since you are looking for Constant variables, click the **Specification** column header again.

Now the variables specified as Constant appear first. The two variables you will select are near the top of the list.

6 Click the C2S.D.STR.C2H6 variable to select it. Then press and hold the Control key and click the C2S.B.STR.C2H4 variable to select both variables.

The selected variables are highlighted.

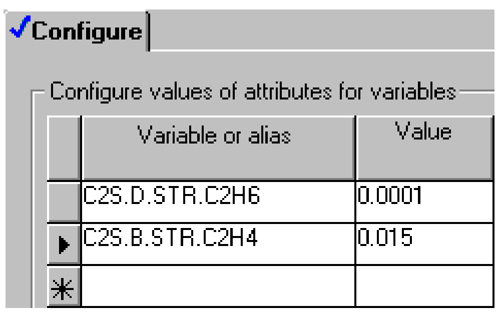
7 Click **Select**.

The selected variables are copied to the **EO Input Configure** sheet.

8 Enter these values for the variables:

Variable	Value
C2S.D.STR.C2H6	0.0001
C2S.B.STR.C2H4	0.015

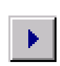
Later in this chapter, you will use this same sheet to specify upper and lower bounds for these variables for an optimization run.



Running the Simulation

Run the EO Simulation

1 Go to the **Control Panel**.

2 In the Control Panel toolbar, click  to run the simulation. Since EO is now running with different specifications than SM, the solver must iterate a few times.

The Control Panel displays the following information for the current run:

```
           Residual   Objective   Objective    Overall       Model
         Convergence Convergence  Function  Nonlinearity Nonlinearity  Worst
Iteration   Function    Function     Value       Ratio        Ratio     Model
--------- ----------- ----------- ---------- ------------ ------------ --------
      0      4.150D+01   0.000D+00  0.000D+00    2.150D-01    2.150D-01 C2S
      1      4.429D-01   0.000D+00  0.000D+00    6.806D-01    6.806D-01 C2S
      2      1.421D-01   0.000D+00  0.000D+00    7.116D-01    7.116D-01 C2S
      3      2.165D-02   0.000D+00  0.000D+00    9.002D-01    9.002D-01 C2S
      4      4.103D-04   0.000D+00  0.000D+00    9.906D-01    9.906D-01 C2S
      5      5.037D-08   0.000D+00  0.000D+00

Successful solution.


Optimization Timing Statistics         Time      Percent
================================      ========   =======

MODEL computations                    0.55 secs    77.46 %
DMO computations                      0.08 secs    11.27 %
Miscellaneous                         0.08 secs    11.27 %
--------------------------------     ---------    -------
Total Optimization Time               0.71 secs   100.00 %

Problem converged
```

Now that you have made changes to the EO simulation, the current problem statement of the SM simulation is not identical to the current problem statement of the EO simulation.

After every EO solution run, the EO results are used to update the results forms. Therefore, you can view the results of this simulation either in the Aspen Plus results forms or in the **EO Variables** form.

3 Go to the **EO Configuration | EO Variables** form.

4 Double-click the **Specification** column header twice to bring the Constant variables to the top.

Index	Variable	Value	Units	Specification
14	C2S.D.STR.C2H6	0.0001	FRACTION	Constant
20	C2S.B.STR.C2H4	0.015	FRACTION	Constant
41	C2S.BLK.EFF_1	0.9	UNITLESS	Constant
1251	C2S.BLK.PSPEC_1	20	BAR	Constant
1252	C2S.BLK.PSPEC_2	20.5	BAR	Constant
1253	C2S.BLK.PSPEC_60	21	BAR	Constant
1254	C2S.BLK.PSPEC_100	21.5	BAR	Constant
1259	F.BLK.MASS	50000	KG/HR	Constant
1262	F.BLK.C2H4_MOLE_FRAC	0.8	FRACTION	Constant
1263	F.BLK.C2H6_MOLE_FRAC	0.2	FRACTION	Constant
1266	F.BLK.TEMP	25	C	Constant
1267	F.BLK.PRES	25	BAR	Constant
1272	F.BLK.SUM	1	FRACTION	Constant

5 Scroll to the bottom of the list to examine the Calculated distillate mass flow and reflux ratio.

Index	Variable	Value	Units	Specification
1233	C2S.BLK.DISTILLATE_MOLE	1400.42	KMOL/HR	Calculated
1234	C2S.BLK.DISTILLATE_MASS	39287.4	KG/HR	Calculated
1235	C2S.BLK.DISTILLATE_STDV	118.632	CUM/HR	Calculated
1236	C2S.BLK.BOTTOMS_MOLE	356.617	KMOL/HR	Calculated
1237	C2S.BLK.BOTTOMS_MASS	10712.6	KG/HR	Calculated
1238	C2S.BLK.BOTTOMS_STDV	30.2096	CUM/HR	Calculated
1239	C2S.BLK.REFL_RATIO_MOLE	3.51278	UNITLESS	Calculated
1240	C2S.BLK.REFL_RATIO_MASS	3.51278	UNITLESS	Calculated
1241	C2S.BLK.REFL_RATIO_STDV	3.51278	UNITLESS	Calculated

6 Go to the **Results Summary | Streams | Material** sheet to examine the results reported there.

Material | Heat | Load | Work | Vol.% Curves | Wt. % Curves | Petro. Cur

Display: All streams Format: GEN_M Stream Table

	B	D	F
Temperature C	-5.2	-29.2	25.0
Pressure bar	21.500	20.000	25.000
Vapor Frac	0.000	0.000	1.000
Mole Flow kmol/hr	356.617	1400.393	1757.041
Mass Flow kg/hr	10712.573	39286.569	50000.000
Volume Flow cum/hr	28.051	95.389	1448.677
Enthalpy MMkcal/hr	-8.070	13.242	10.032
Mass Flow kg/hr			
C2H4	150.067	39282.358	39433.283
C2H6	10562.506	4.211	10566.717
Mole Flow kmol/hr			
C2H4	5.349	1400.253	1405.633
C2H6	351.268	0.140	351.408
Mole Frac			
C2H4	0.015	1.000	0.800
C2H6	0.985	100 PPM	0.200

Note: The original input values for distillate flow rate and reflux ratio you specified on the **Blocks | C2S | Setup | Configuration** sheet are intact, in case you want to perform another SM run.

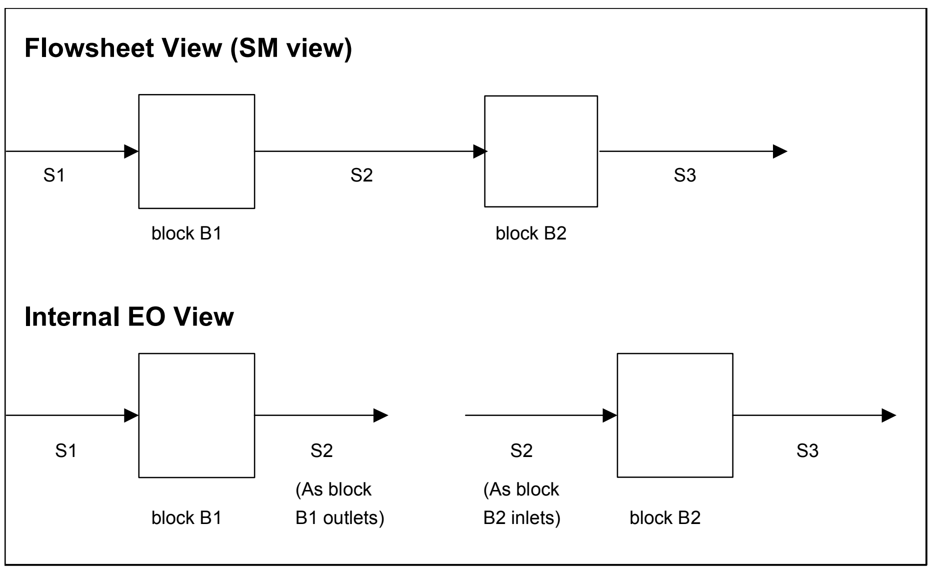
Notice that there is a set of variables for the feed stream in the feed block, F, and an identical set in the column block, C2S. Although this may appear redundant, it is actually more effective for the EO system.

The equivalent variables are:

Feed Variable	Tower Variable	Description
F.BLK.MOLES	C2S.F.STR.MOLES	Stream molar flow
F.BLK.TEMP	C2S.F.STR.TEMP	Stream temperature
F.BLK.PRES	C2S.F.STR.PRES	Stream pressure
F.BLK.ENTH	C2S.F.STR.ENTH	Stream specific enthalpy
F.BLK.MVOL	C2S.F.STR.MVOL	Stream molar volume
F.BLK.C2H4	C2S.F.STR.C2H4	Stream ethylene mole fraction
F.BLK.C2H6	C2S.F.STR.C2H6	Stream ethane mole fraction

Consider the generalized case below. In the SM representation, there are variables associated with streams and variables associated with blocks. Some of the stream variables and block variables may be equivalent, but most are not.

In the EO representation, there are no stream variables. Instead, the variables associated with stream S2 are included as block variables in both blocks, as illustrated in the following figure:



The two representations of the streams are forced to be equal to one another through connection equations. These connection equations are added to the EO representation of the flowsheet automatically.

Feed blocks are used to hold the data for feed streams to a process.

Running an EO Optimization

Now you will attempt a simple optimization problem. To do this, you must:

- Define an objective function
- Select variables
- Set variable bounds

For this example, you will use the linear objective function. As the name implies, this is a simple summation of variable values multiplied by costs:

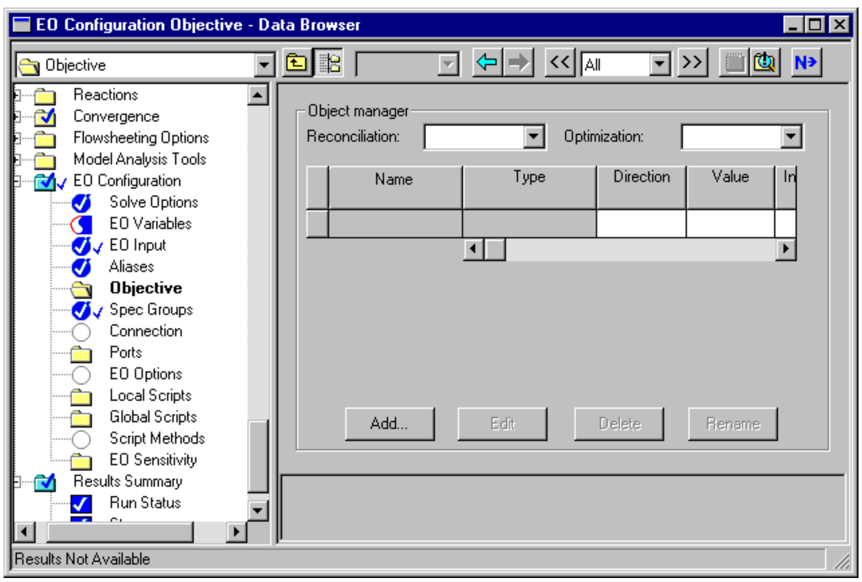
Objective = Σ Variable * Cost

The cost must be a constant term.

Define An Objective Function

1 Click the **EO Configuration | Objective** folder.

The EO Configuration | Objective object manager appears:



2 Click **Add** to add a new objective function.

The **Create new ID** dialog box appears.

3 Enter **PROFIT** as the ID.

4 Select **LINEAR** as the type.

Note: This objective function could be specified as custom, but the optimization algorithm can take a more efficient path if it knows the objective is linear.

5 Click **OK**.

The **EO Configuration | Objective | PROFIT | Input | Setup** sheet appears.

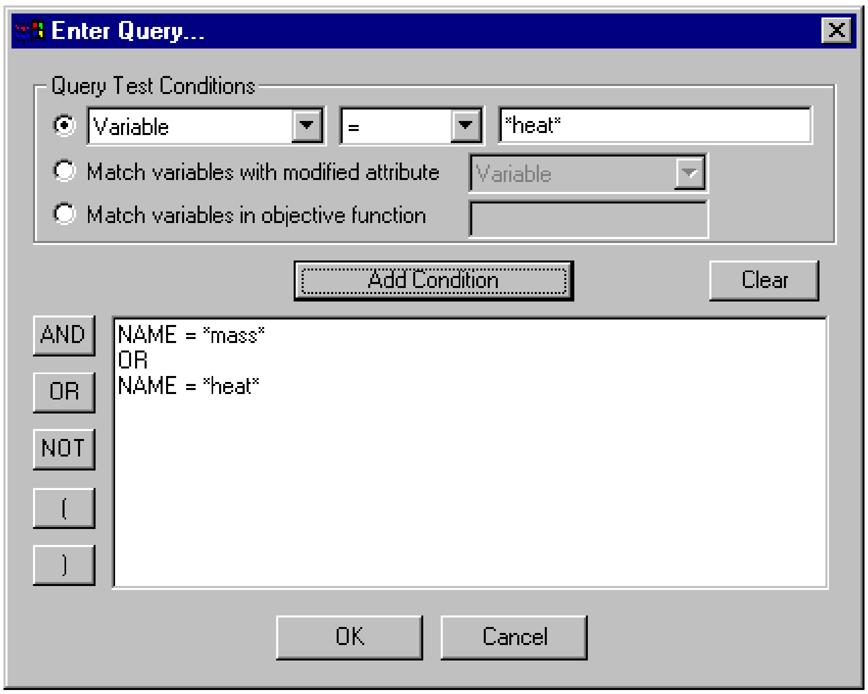
6 In the **Units** field, enter **$/HR**.

7 Click the **Variable / Alias / Objective** field, then click to use the **EO Variables** dialog box to select the variables. In the dialog box, click **Query**. The **Enter Query** dialog box appears.

8 **Variable** and **=** should be selected in the first two fields. Enter *mass* in the third field, and click **Add Condition**.

9 The text NAME = *mass* appears in the query condition box. Click **OR** to the left of this area.

10 Where you entered *mass* before, change it to *heat*. Click **Add Condition**.



11 Click **OK**. The EO Variables dialog box now lists only variables whose names contain *mass* or *heat*.

12 Hold down the Control key on the keyboard and click the names of the three variables listed below. Click **Select**. These names are copied to the objective function form.

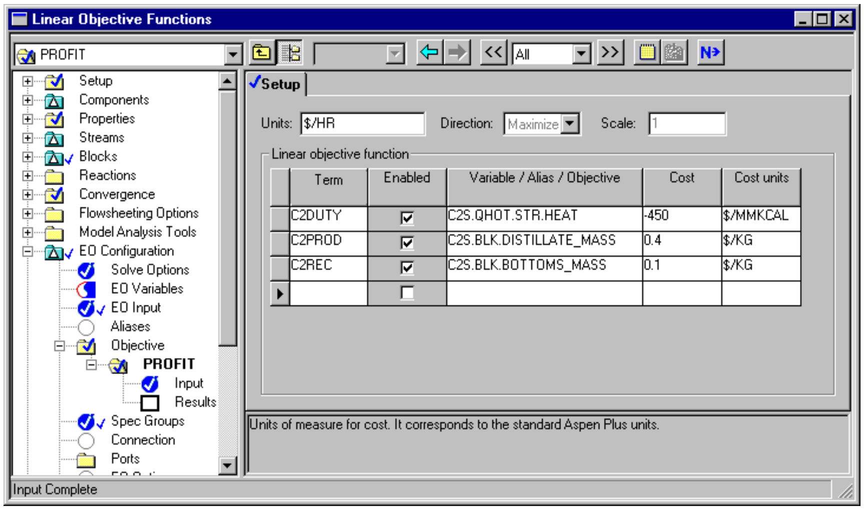
Term	Variable	Cost	Units
C2PROD	C2S.BLK.DISTILLATE_MASS	0.4	$/KG
C2REC	C2S.BLK.BOTTOMS_MASS	0.1	$/KG
C2DUTY	C2S.QHOT.STR.HEAT	-450.	$/MMKCAL

13 Enter the rest of the data above into the Term, Cost, and Units fields on the form. Note that the variables might not appear in this order.

These three terms represent the value of the two tower products and the cost of the condenser duty. Although there is a cost for the feed, it is not included in this example objective function because the feed rate is not a degree of freedom.

The **Direction** defaults to **Maximize** for linear objective functions, which is what we want.

The EO Configuration | Objective | PROFIT | Input | Setup sheet is complete:



This completes the definition of the objective function. Based upon these prices, revenue is received for the distillate and bottoms streams and a cost is paid for the condenser duty. Since the distillate stream is the desired product, it is valued significantly higher than the bottoms. The total profit in dollars per hour is:

C2PROD*0.4 + C2REC*0.1 – C2DUTY*450 ≈ 10,566 $/HR.

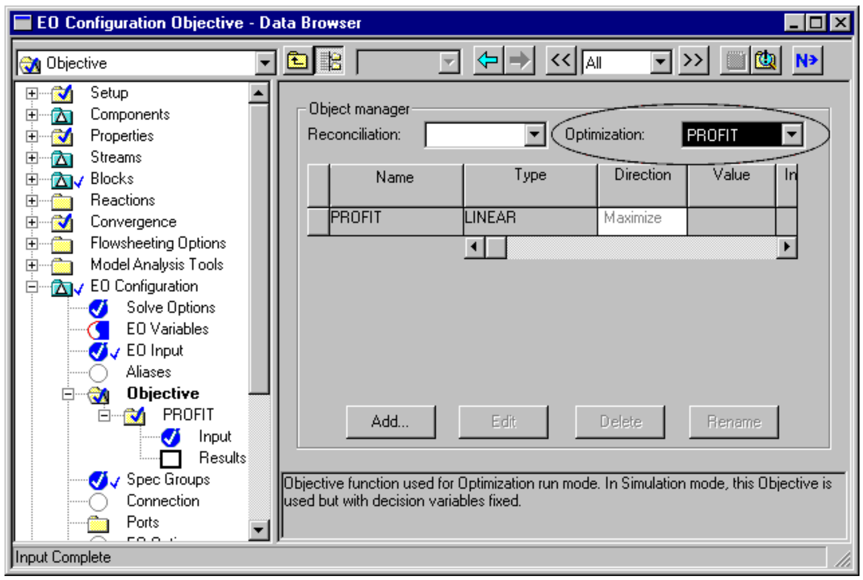
The concentrations of ethane and ethylene in the distillate and bottoms product stream will be varied within specified bounds to maximize this profit objective function.

Select the Objective Function

You have defined the objective function, PROFIT. However, before you can use it in an EO Reconciliation or Optimization run, you must select it.

1 Click the **EO Configuration | Objective** folder.

2 In the **Optimization** field, select **PROFIT**.



The objective function is now set to PROFIT when the problem is run in the EO Optimization mode. In this case, there is only one objective function. However, you could define several and pick the one you want for a particular optimization run.

Now define the variables that will be degrees of freedom during the Optimization run. The distillate and bottoms ethane and ethylene concentrations currently specified as Constant in the C2COMPS Spec Group must now be specified as Optimized.

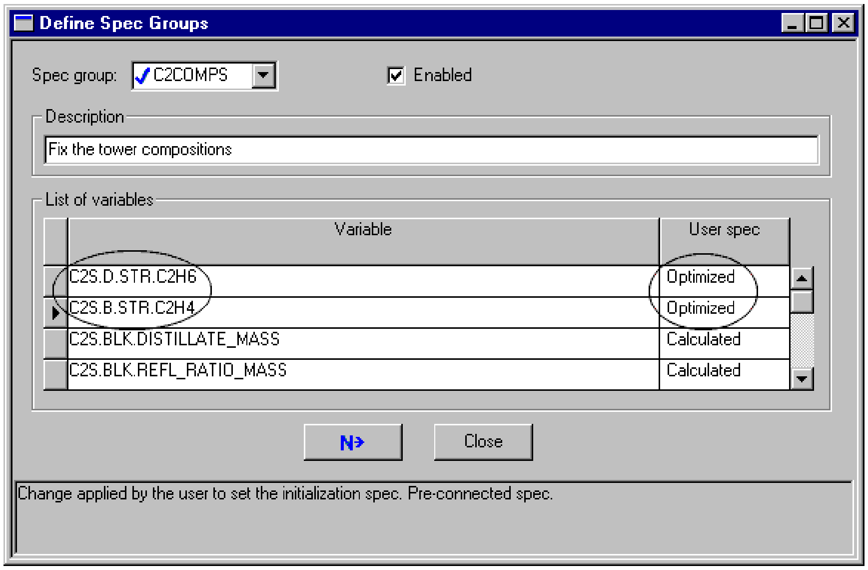
Select the Independent Variables

1 Go to the **EO Configuration | Spec Groups | Specifications** sheet.

2 Select **C2COMPS** and click **Edit**.

The **Define Spec Groups** dialog box appears.

3 Change the **User spec** from **Constant** to **Optimized** for the two compositions: C2S.D.STR.C2H6 and C2S.B.STR.C2H**4**



4 Click **Close** to close the dialog box.

You could run the simulation now even though ranges have not been set for the two product stream variables and the Solution Mode has not been set to Optimization. The two product stream variables are still Fixed in Simulation mode. They are only DOF variables during Optimization runs.

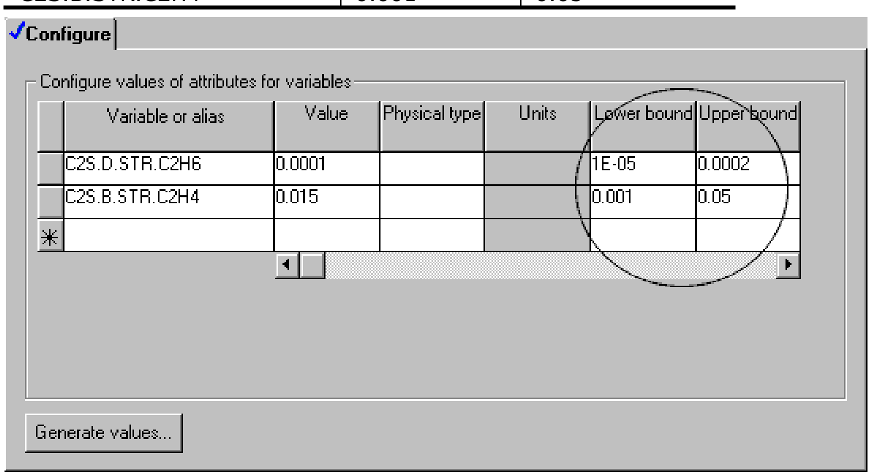
The last thing to do is to set upper and lower limits over which Aspen Plus is allowed to vary the two concentrations.

Set Bounds for the Independent Variables

1 Go to the **EO Configuration | EO Input** form.

2 Enter the following values for the variable bounds:

Variable	Lower	Upper
C2S.D.STR.C2H6	0.00001	0.0002
C2S.B.STR.C2H4	0.001	0.05

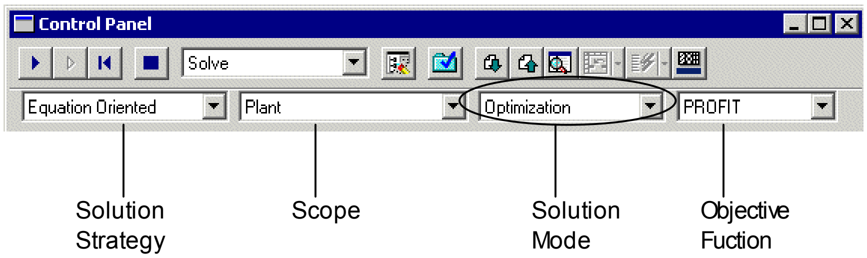


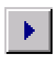
Run the Simulation in Optimization Mode

1 Open the **Control Panel**.

2 In the **Solution mode** field, select **Optimization**.

3 Verify that the **Objective function** is set to **PROFIT**.



4 Click  to run the optimization.

This solution requires several iterations of the solver while it seeks the optimum operating conditions. The value and convergence status of the objective function appears in the Control Panel output for each iteration.

View the Optimization Results

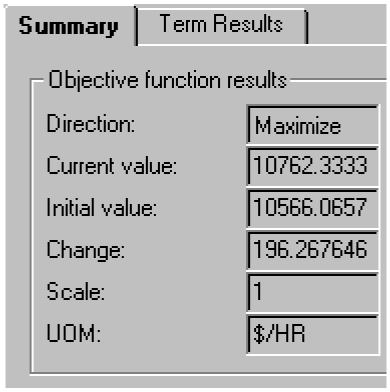
1 Go to the **EO Configuration | EO Variables** form.

2 Double-click twice on the **Specification** column header to display the optimized and constant variables.

Index	Variable	Value	Units	Specification
14	C2S.D.STR.C2H6	0.0002	FRACTION	Optimized
20	C2S.B.STR.C2H4	0.00729651	FRACTION	Optimized
41	C2S.BLK.EFF_1	0.9	UNITLESS	Constant
1251	C2S.BLK.PSPEC_1	20	BAR	Constant
1252	C2S.BLK.PSPEC_2	20.5	BAR	Constant
1253	C2S.BLK.PSPEC_60	21	BAR	Constant
1254	C2S.BLK.PSPEC_100	21.5	BAR	Constant
1259	F.BLK.MASS	50000	KG/HR	Constant
1262	F.BLK.C2H4_MOLE_FRAC	0.8	FRACTION	Constant
1263	F.BLK.C2H6_MOLE_FRAC	0.2	FRACTION	Constant
1266	F.BLK.TEMP	25	C	Constant
1267	F.BLK.PRES	25	BAR	Constant
1272	F.BLK.SUM	1	FRACTION	Constant

As expected, the composition of ethane in the more-profitable distillate is now at its upper bound of 0.0002. Because it is at the limit, the upper bound attribute in the EO variable grid is blue.

3 Go to the **EO Configuration | Objective | PROFIT | Results** sheet to see the maximized profit result.



4 Save the simulation and exit from Aspen Plus.

Note: This simulation is delivered as a backup file, **eogsg1**, in the Aspen Plus Examples Library. Use this backup file to check your results.

2 Heat Integration

This session continues where the previous session ended. To demonstrate heat integration, you will add an HXFlux block and a Heater block to model the condenser. Propylene is used as the refrigerant on the utility side of the condenser.

You will use this configuration to perform a more accurate economic optimization based on the refrigerant cost and flow rate required rather than on an estimated heat duty cost.

In this session you will:

- Set up a utility stream.
- Define an HXFlux model and heat-integrate the utility stream and the column.
- Define connections between variables.
- Use component groups to control the components used in each section of the EO simulation.
- Change some variable specifications and other attributes.
- Perform an economic optimization.

Allow about 45 minutes to do this simulation.

Modeling the Condenser

Add two unit operation models to the Process Flowsheet to model the condenser, include propylene as a component available to the simulation, set up two groups of components that will be used later to improve the performance of the EO solver, specify the characteristics of the coolant feed stream, and configure the two new blocks.

Build the Process Flowsheet

1 Open the simulation file from the previous chapter, **EO1.apw**.

   The HXFlux/Heater combination is used to model the column condenser.

2 In the **Model Library**, click the **Heat Exchangers** tab.

3 Click the arrow next to the **Heater** block and select the **HEATER** icon.

4 Place the block on the Process Flowsheet.

   The **Input** dialog box appears.

5 Name the block **CVAP**.

6 On the Process Flowsheet, connect a feed stream to the **CVAP** block and name the stream **CIN**.

7 Connect a product stream to the **CVAP** block and name it **COUT**.

8 In the Model Library, select the **HXFlux** model and place an **HXFlux** block on the Process Flowsheet.

   The **Input** dialog box appears.

9 Name the block **CONDUA**.

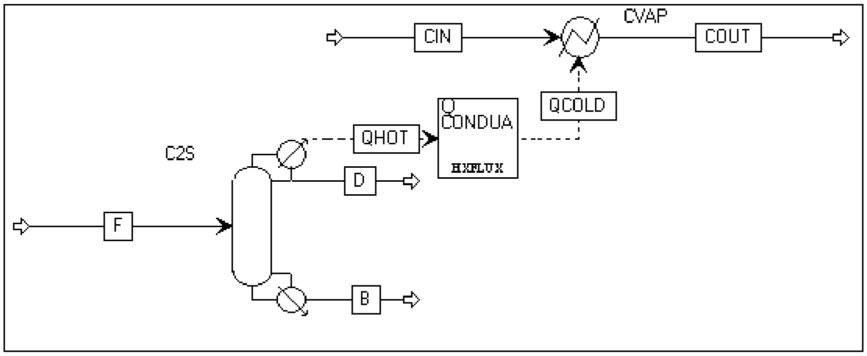
10 On the flowsheet, connect a heat stream, named **QCOLD**, from the **CONDUA** block to the **CVAP** block.

11 Select **QHOT** heat stream, right-click to display the shortcut menu, and select **Reconnect Destination**.

12 Connect the **QHOT** heat stream as an inlet to the **CONDUA** block.

Note: The look of the drawing may be changed by selecting a block and then selecting the blue port stream indicators. You can move the port indicator to other locations on the block.

The Process Flowsheet should look like this:



The coolant used for the **CIN** and **COUT** coolant stream in this example will be propylene. Add it to ethylene and ethane on the **Components | Specifications | Selection** sheet.

Specify Propylene as a Component in the Simulation

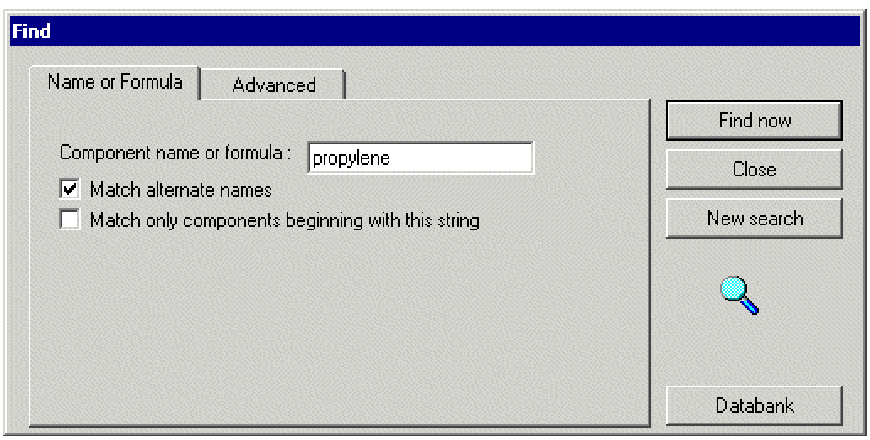
1 On the Aspen Plus toolbar, click  to open the Data Browser.

2 Go to the **Components | Specifications | Selection** sheet.

3 Click **Find**.

The **Find** dialog box appears.

4 In the **Component name or formula** field, enter **Propylene**.



5 Click **Find Now**.

The list of possible components appears in the dialog box.

6 Select **PROPYLENE** and click **Add**.

7 Click **Close**.

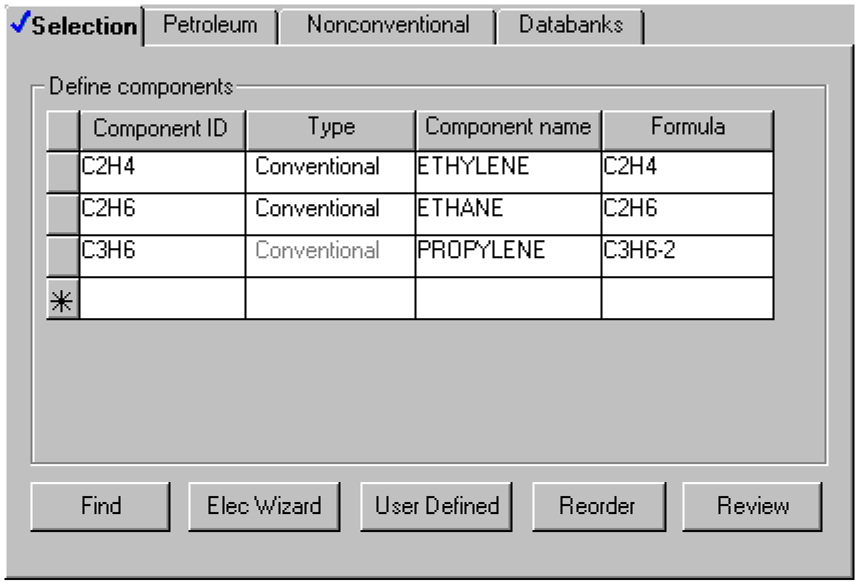
Propylene is now available to the simulation under the ID PROPY-01.

8 In the **Component ID** field select **PROPY-01**, type **C3H6** in its place, and press **Enter** on the keyboard.

An **Aspen Plus** dialog box appears.

9 Click **Rename**.

Propylene can now be referred to as **C3H6** in this simulation.



Next specify the coolant feed stream (**CIN**) characteristics. It will consist of propylene with a vapor fraction of zero. The flow rate will be specified. In the EO simulation, the flow rate will be calculated based on the condition that all of the propylene is vaporized.

Specify Coolant Feed Stream Characteristics

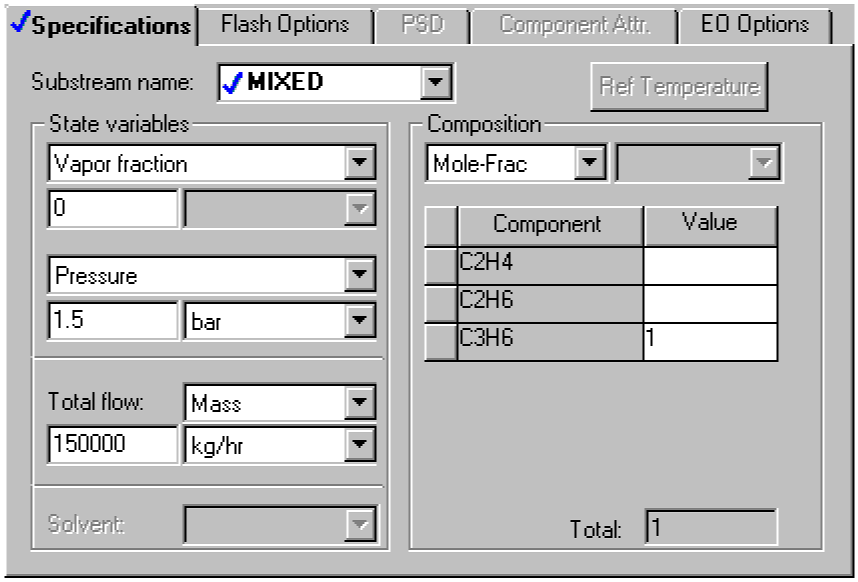
1 Go to the **Stream | CIN | Input | Specifications** sheet and change the State variable, **Temperature** to **Vapor Fraction**.

2 In the first State variable field, change **Temperature** to **Vapor fraction**, and enter the following values:

Field	Value
Vapor fraction	0
Pressure	1.5 Bar
Total flow	Mass 150,000 kg/hr
Composition	Mole-Frac
Component C3H6	1.0

Note: These specifications make the vapor fraction, pressure, total mass flow, and propylene mole fraction variables Constant in EO.

The **Streams CIN Input Specifications** sheet is complete:



Next, configure the two new blocks.

For the **CONDUA** block, specify the heat transfer coefficient and estimate the hot stream and cold stream temperatures needed to calculate the LMTD. Aspen Plus will use these data to calculate the required heat transfer area.

For the **CVAP** block, only the pressure drop needs to be specified.

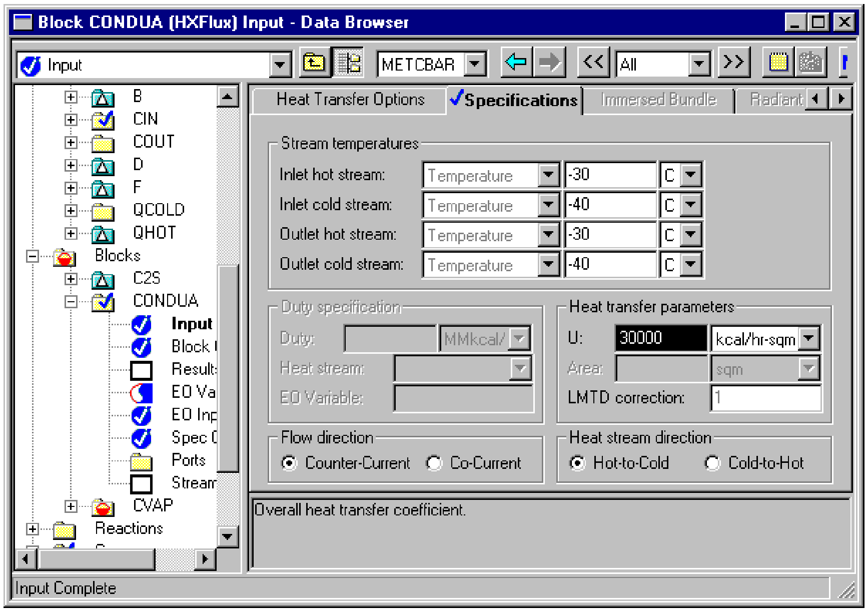
Configure the CONDUA and CVAP Blocks

1 In the **Blocks | CONDUA | Input | Specifications** sheet, enter the following values for the Stream Temperatures:

Field	Value 1	Value 2
Inlet hot stream	Temperature	-30
Inlet cold stream	Temperature	-40
Outlet hot stream	Temperature	-30
Outlet cold stream	Temperature	-40

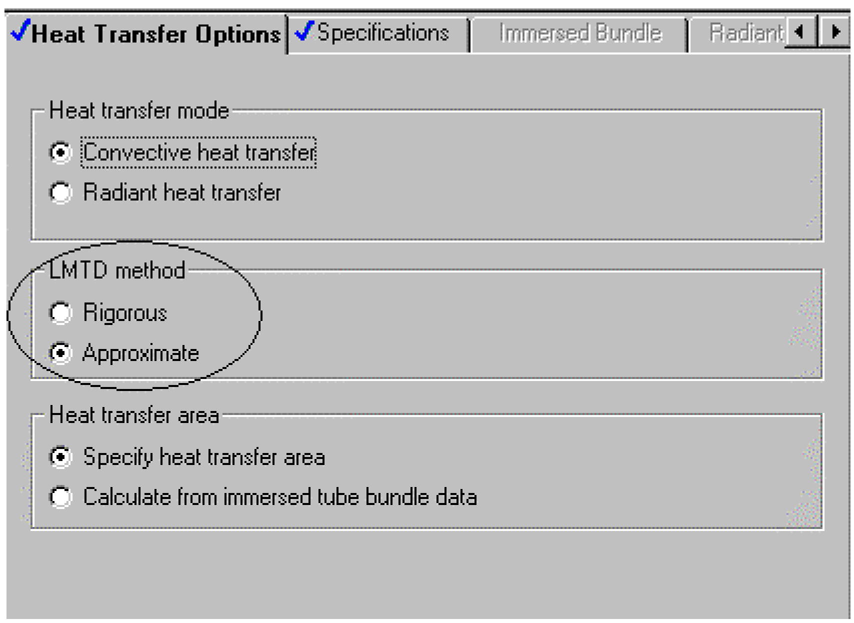
Note: On this sheet, you can select **Temperature**, **Stream**, or **EO Variable** from the dropdown lists in the Stream temperatures area. You would typically refer to Stream or EO Variables to set the temperatures rather than supplying numerical estimates. In this example, this reference will be accomplished via user-defined connections between EO variables in order to illustrate this feature of Aspen Plus EO modeling.

2 In the Heat transfer parameters area, enter **30,000 Kcal/hr sqm K** in the **U** field.



3 Click the **Heat Transfer Options** tab.

4 In the LMTD method area, select **Approximate**.

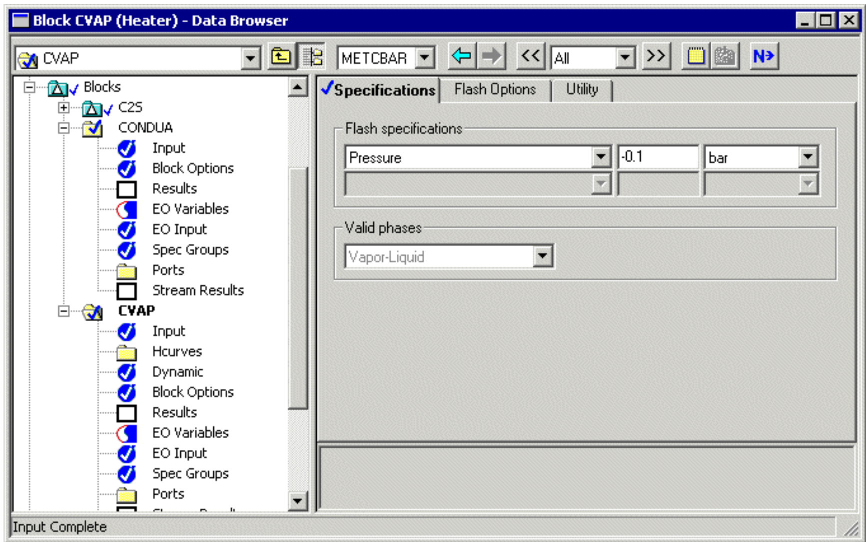


Selecting the approximate option for the LMTD method avoids potential numerical difficulties with the rigorous form of EO formulation. For more information on the differences between the Rigorous and Approximate LMTD method, see the Online Help.

5 Go to the **Blocks | CVAP | Input | Specifications** sheet.

6 In the Pressure field enter **-0.1 bar**.

This value gives the heater block a small pressure drop and makes pressure drop Constant in EO.



The SM flowsheet configuration is complete.

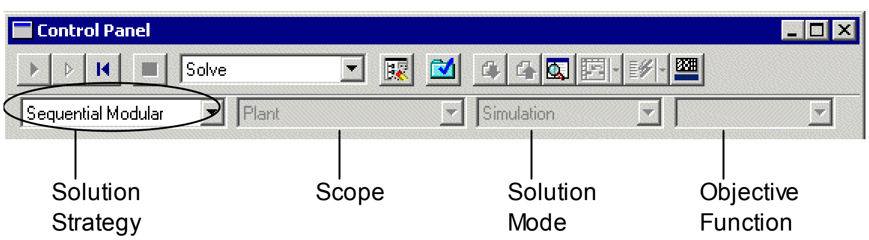
7 Save the simulation file as **EO2apw**.

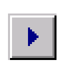
Running the Simulation

First, solve this simulation with the Sequential Modular (SM) strategy. The SM input values for the Feed stream composition and flow rate and for the distillate flow rate and reflux ratio are unchanged from the previous chapter, so you will get the same results.

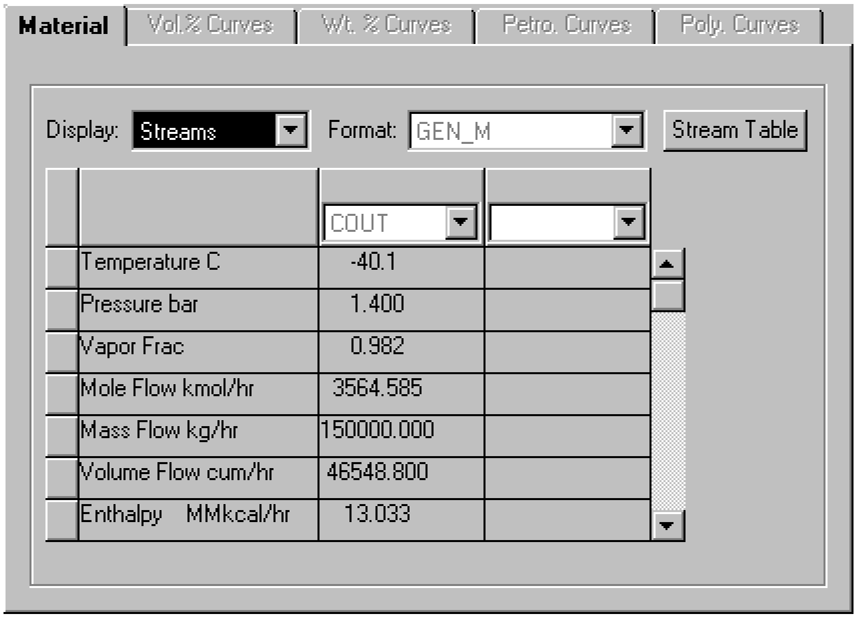
1 Go to the **Control Panel**.

2 In the **Solution Strategy** field, select **Sequential Modular**.



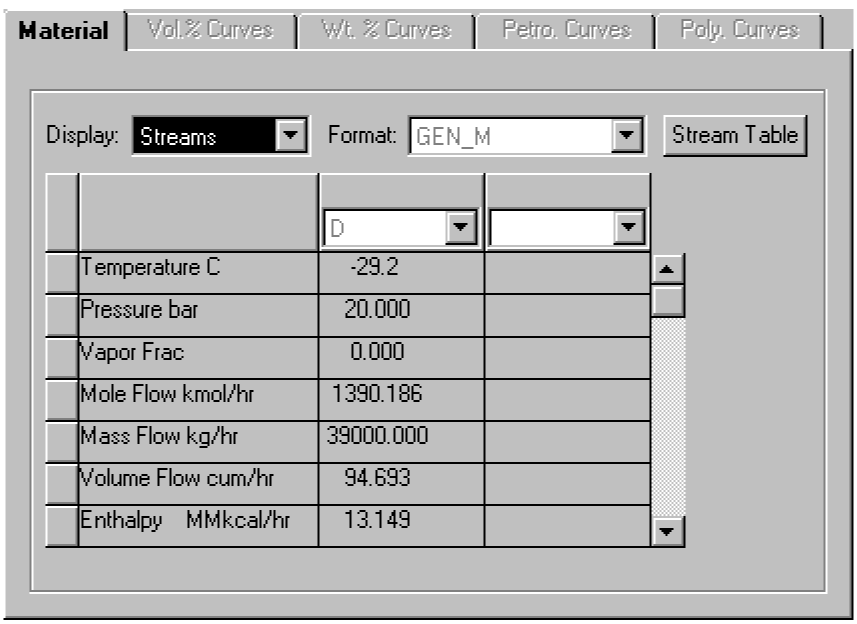
3 On the Control Panel toolbar, click  to run the simulation.

4 Go to the **Streams | COUT | Results Material** sheet.



Not all of the coolant was vaporized, and the actual boiling point of the propylene stream is –40.1 C rather than –40 C.

5 Go to the **Streams | D | Results Material** sheet.



The actual temperature of the condensed distillate is –29.2 C rather than –30 C.

In the EO simulation, these more accurate temperatures will be used, the vapor fraction of the COUT stream will be set at 1.0, and the flow rate of the COUT stream will be calculated rather than estimated.

Running an EO Simulation

Before you run the EO simulation, you will make some input changes. In the following sections, you will:

- Create two flowsheet sections and two component groups and assign a component group to each section.
- Specify the COUT vapor fraction as Constant and the CIN flow rate as Calculated.
- Define user connections so that more accurate temperatures are used in the CONDUA block and view these connections on the Process Flowsheet.

In the Sequential Modular (SM) solution strategy, extra components with zero flow have little effect on performance because each unit operation can filter out the null components before executing. In the Equation Oriented (EO) solution strategy, however, every component adds variables and equations to the overall problem. This increases the size of the problem and leads to increased memory requirements and longer solution time. Therefore, there is generally an incentive to reduce the open model component slate whenever possible.

The ability to specify nonzero components allows you to achieve this goal. One way to do this is to assign component groups, representing the nonzero components, to flowsheet sections. In this example, there will be two component groups – one containing ethylene and ethane and another containing propylene. You will create two flowsheet sections – one corresponding to the C2S block and one corresponding to the CVAP block. Then you will assign each component group to the appropriate section.

Create Two Component Groups

1 In the Data Browser menu tree, click the **Components | Comp-Groups** folder.

The **Components | Comp-Groups** object manager appears.

2 Click **New**.

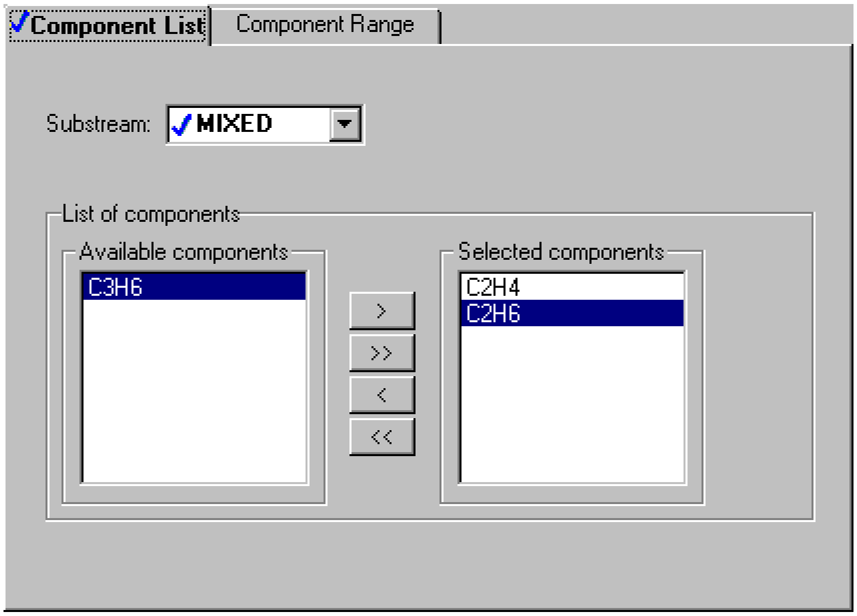
The **Create new ID** dialog box appears.

3 Enter **C2GROUP** as the ID and click **OK**.

The **Components | Comp-Groups | C2GROUP | Component List** sheet appears in the Data Browser.

4 In the **Available components** column, select **C2H4** and click  to move it into the **Selected components** column.

5 Move C2H6 into the Selected components column.



6 Use the Data Browser menu tree to go back to the **Components | Comp-Groups** object manager.

7 Click **New** to create another component group. Name this one **C3GROUP** and place **C3H6** in the **Selected components** column.

Next, create two flowsheet sections corresponding to the C2S block and the CVAP block.

Create Two Flowsheet Sections

1 In the Process Flowsheet, select the **C2S** block, then right-click to display the shortcut menu, and choose **Change Section**.

The **Change Section** dialog box appears.

2 Select **Create New Section** and enter the name, **C2SECT**.

3 Click **OK**.

4 Create a section called **C3SECT** for the **CVAP** block (repeat steps 1 – 3).

Now, there are three flowsheet sections:

- **C2SECT**, which holds the **RadFrac** block **C2S**.
- **C3SECT**, which holds the **Heater** block **CVAP**.
- **GLOBAL**, which holds the **HXFlux** block **CONDUA**.

There are several mechanisms for assigning component groups. A component group may be assigned globally, to a particular flowsheet section or to an individual block. For a block containing multiple models, a component group can be assigned to a particular model.

Here, you will assign the component groups at the flowsheet section level.

Assign Component Groups

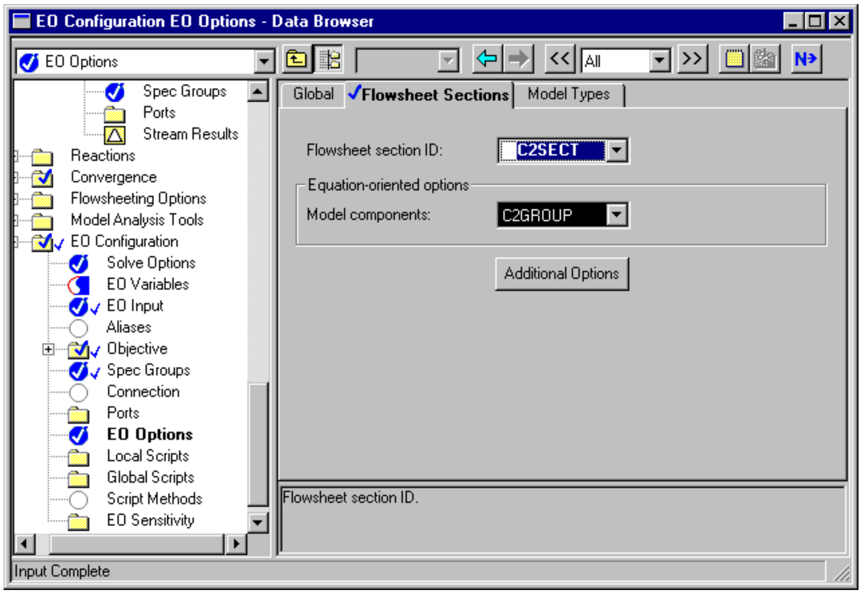
1 Go to the **EO Configuration | EO Options** form.

2 Click the **Flowsheet Sections** tab.

3 In the **Flowsheet section ID** field, select **C2SECT**.

4 In the **Model components** field, select **C2GROUP**.

This assigns the **C2GROUP** component group to the flowsheet section **C2SECT**.



5 In the **Flowsheet Section ID** field, select **C3SECT**.

6 In the **Model Components field**, select **C3GROUP**.

The specification of model components (component groups) is not required. In many cases, failure to specify model components increases the memory and time required to run the EO simulation, but does not affect the overall EO convergence behavior and does not cause a noticeable increase in execution time. But in other cases, convergence may be adversely effected or there may be a noticeable reduction in speed.

The specification of model components may also help to eliminate physical property error messages pertaining to components that are not present.

Next, change the variable specifications so that the EO simulation fixes the outlet propylene stream at its dew point and computes the required flow. Implement these changes as a Spec Group.

Define a Spec Group

1 Go to the **EO Configuration | Spec Groups | Specifications** sheet.

2 In the first blank row under the **Spec group** column, type **C3RVFRAC** and press **Enter** on the keyboard.

3 Select the C3RVFRAC row and click Edit.

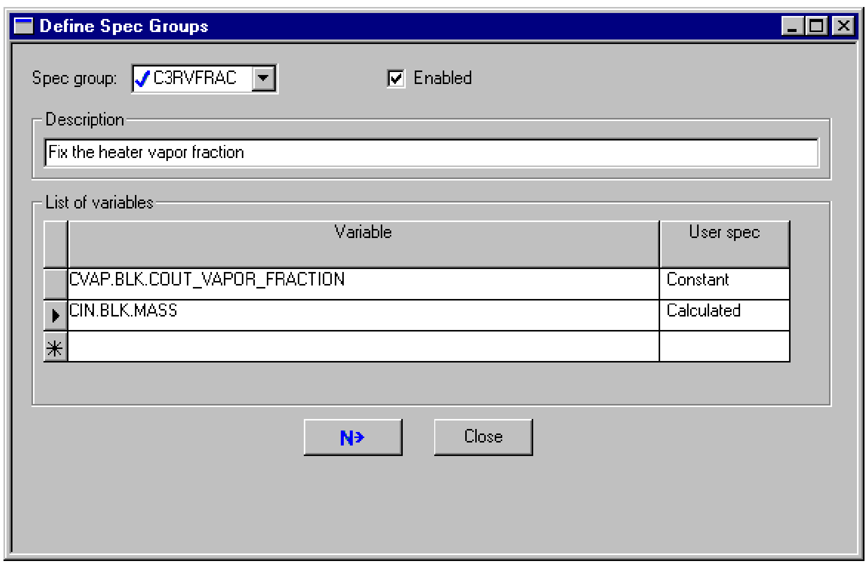
The **Define Spec Groups** dialog box appears.

4 In the **Description** field, type: *Fix the heater vapor fraction*.

5 Enter the following variable names and user specs:

Variable	User Spec
CVAP.BLK.COUT_VAPOR_FRACTION	Constant
CIN.BLK.MASS	Calculated

6 Verify that the **Enabled** checkbox is selected.



7 Click **Close**.

Next, set the COUT vapor fraction (now a Constant EO variable) to 1.0. You do not want to use the value of CVAP.BLK.COUT_VAPOR _FRACTION calculated from the last simulation as the constant value, so you need to specify a value for this variable.

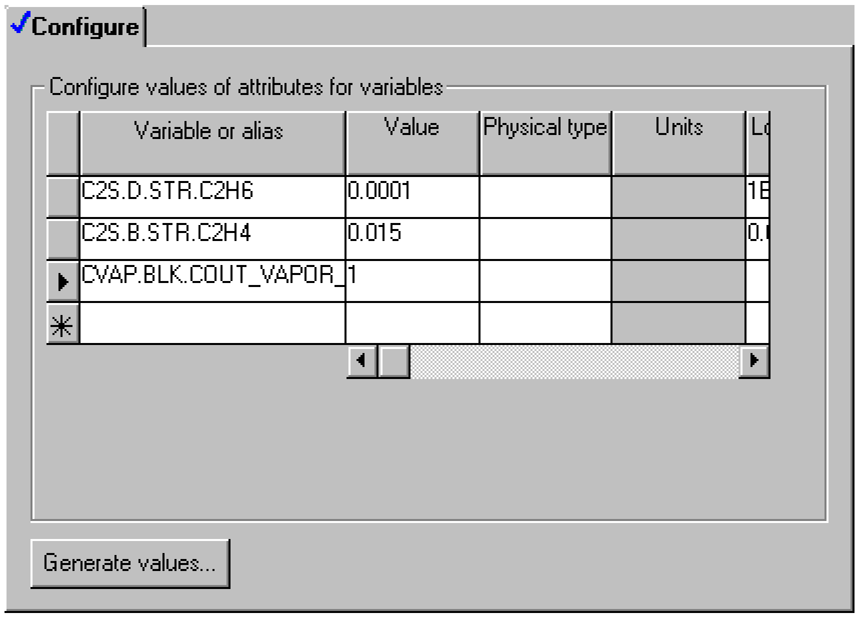
In general, whenever a variable specification is flipped from Calculated to Constant, you should consider how that variable will be set.

Specify the COUT Vapor Fraction

1 Go to the **EO Configuration | EO Input | Configure** sheet.

2 In the first available row, enter the following:

Variable or alias	Value
CVAP.BLK.COUT_VAPOR_FRACTION	1



Next, define user connections between the temperature variables so that the HXFlux model uses more accurate temperatures.

The HXFlux model requires inlet and outlet temperatures for the hot and cold sides to evaluate the log mean temperature difference. Originally, constant values were entered in the HXFlux configuration and used for the SM run.

To truly heat-integrate the processes, you need to define User Connections between the HXFlux block and the source blocks.

Note: The reason User Connections are needed is because stream connections were not used in the original specification of HXFlux. The example was designed this way so that User Connections could be demonstrated.

About Connections

Connections are additional equations that can be added to the system that equate two variables – a *source* and a *destination* – ensuring that they have the same value at the solution.

Connection processing automatically adjusts the specifications of the variables involved in order to preserve the net specification of the problem. Since one equation is added to the system, one specification must be removed, generally by making one Fixed variable Free. Usually, the destination variable is changed from Constant to Calculated.

Connection processing occurs after Spec Group processing, and occurs in three steps. First, stream connections (as discussed in chapter 2) are processed, then user connections are processed, and finally, measurement connections are processed.

In this example, the four temperatures in the HXFlux block were specified as Constant by default. Their values were specified on the **Blocks | CONDUA | Input | Specifications** sheet.

When connections are added to these variables, their specification is automatically changed from Constant to Calculated and four connection equations are added to the problem.

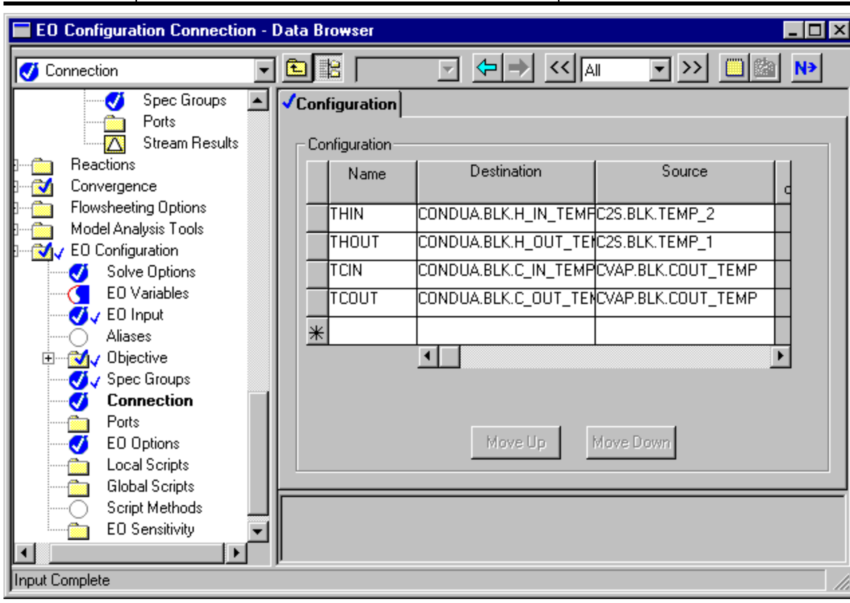
With the HXFlux block configured in this manner, it will compute the required heat transfer area to meet the duty requirements for the temperatures provided.

Define User Connections

1 Go to the **EO Configuration | Connection | Configuration** sheet.

2 Enter the following information:

Name	Destination	Source
THIN	CONDUA.BLK.H_IN_TEMP	C2S.BLK.TEMP_2
THOUT	CONDUA.BLK.H_OUT_TEMP	C2S.BLK.TEMP_1
TCIN	CONDUA.BLK.C_IN_TEMP	CVAP.BLK.COUT_TEMP
TCOUT	CONDUA.BLK.C_OUT_TEMP	CVAP.BLK.COUT_TEMP



This configuration will connect the appropriate temperatures into the CONDUA block. The same temperature is used for the cold stream inlet and outlet, since the majority of the heat transfer is occurring at that temperature.

The user connections should appear on the Process Flowsheet as blue lines labeled with the name of the connection. If they do not appear automatically, follow these steps:

Viewing the Connections on the Flowsheet

1 From the **Aspen Plus** menu bar, choose **Tools | Options**.

The **Options** dialog box appears.

2 Select the **Flowsheet** tab.

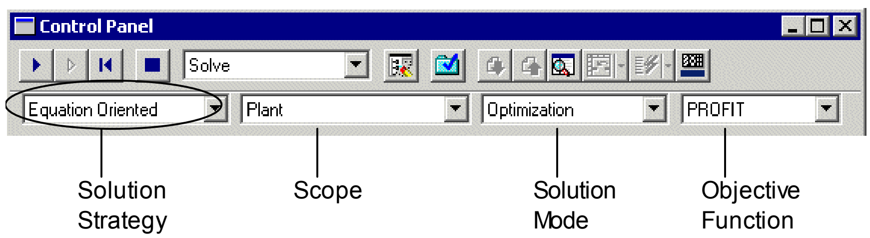
3 Select the **Display connection streams** checkbox.

4 Click **OK** to close the dialog box and apply the change.

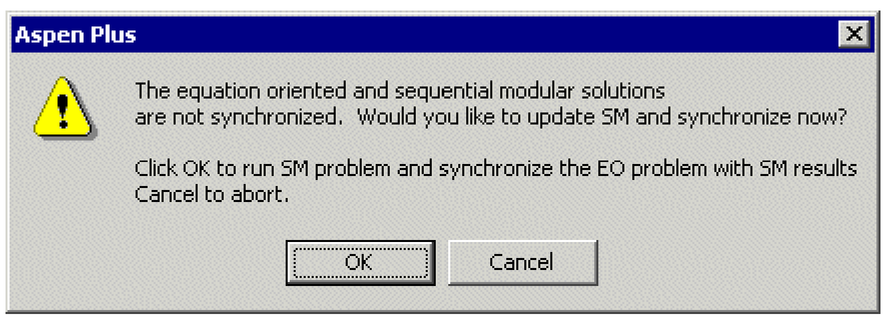
Running the EO Simulation

1 Go to the Control Panel

2 From the **Solution Strategy** list, select **Equation Oriented**.



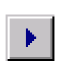
An **Aspen Plus** dialog box appears:



3 Click **OK** to update SM and synchronize.

4 Set the **Solution Mode** to **Simulation**.

5 Clear the **Objective Function** field.

6 Click  to run the simulation.

EO is running with different specifications and values than SM, so the solver must iterate a few times.

View the Results of the EO Simulation

1 Go to the **EO Configuration | EO Variables** form.

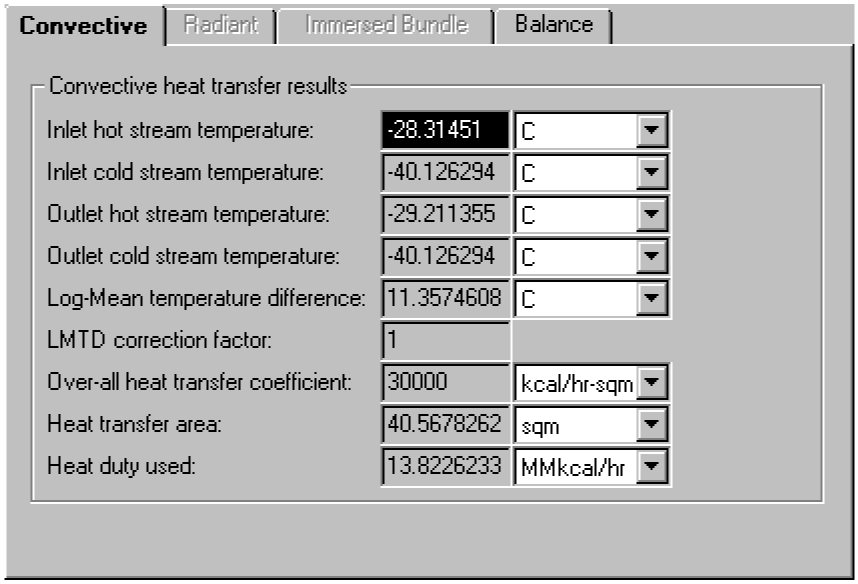
2 Double-click the **Specification** column header twice to bring the Constant variables to the top. Note that the two Optimized variables are Fixed in Simulation mode.

Index	Variable	Value	Units	Specification
14	C2S.D.STR.C2H6	0.0001	FRACTION	Optimized
20	C2S.B.STR.C2H4	0.015	FRACTION	Optimized
41	C2S.BLK.EFF_1	0.9	UNITLESS	Constant
1251	C2S.BLK.PSPEC_1	20	BAR	Constant
1252	C2S.BLK.PSPEC_2	20.5	BAR	Constant
1253	C2S.BLK.PSPEC_60	21	BAR	Constant
1254	C2S.BLK.PSPEC_100	21.5	BAR	Constant
1276	CVAP.BLK.PDROP	0.1	BAR	Constant
1278	CVAP.BLK.COUT_VAPOR_FRACTIO	1	UNITLESS	Constant
1307	CONDUA.BLK.U	30000	KCAL/HR-SQM-	Constant
1308	CONDUA.BLK.FT	1	UNITLESS	Constant
1315	CIN.BLK.C3H6_MOLE_FRAC	1	FRACTION	Constant
1319	CIN.BLK.PRES	1.5	BAR	Constant
1323	CIN.BLK.SUM	1	FRACTION	Constant
1326	CIN.BLK.VAPOR_FRACTION	-9.4e-005	UNITLESS	Constant
1347	F.BLK.MASS	50000	KG/HR	Constant
1350	F.BLK.C2H4_MOLE_FRAC	0.8	FRACTION	Constant
1351	F.BLK.C2H6_MOLE_FRAC	0.2	FRACTION	Constant
1354	F.BLK.TEMP	25	C	Constant
1355	F.BLK.PRES	25	BAR	Constant
1360	F.BLK.SUM	1	FRACTION	Constant

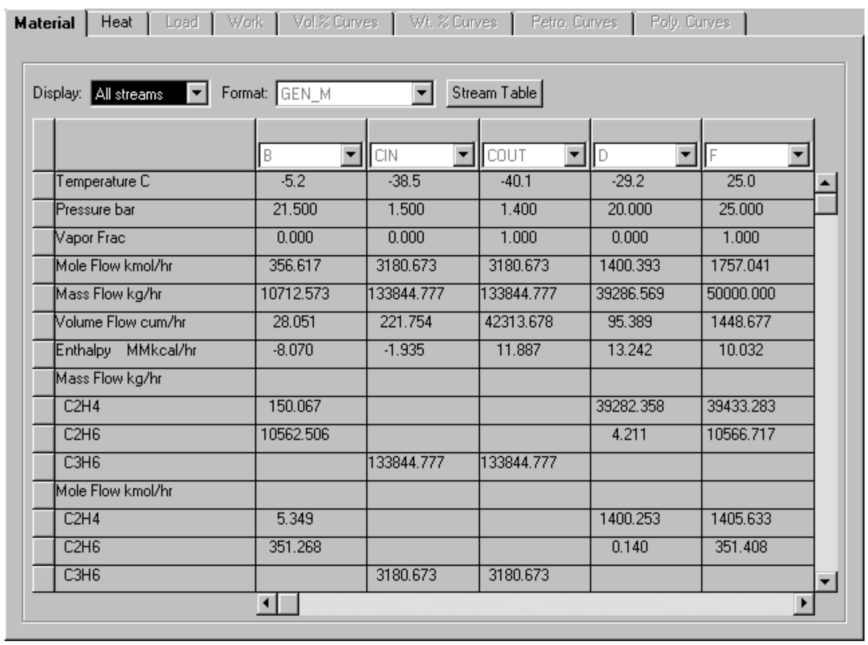
3 Scroll down the variables list to examine some of the relevant Calculated variables.

Index	Variable	Value	Units	Specification
1300	CONDUA.BLK.H_IN_TEMP	-28.3145	C	Calculated
1301	CONDUA.BLK.H_OUT_TEMP	-29.2114	C	Calculated
1302	CONDUA.BLK.C_IN_TEMP	-40.1263	C	Calculated
1303	CONDUA.BLK.C_OUT_TEMP	-40.1263	C	Calculated
1304	CONDUA.BLK.HOT_IN_APPR_TEMP	11.8118	DELTA-C	Calculated
1305	CONDUA.BLK.HOT_OUT_APPR_TEM	10.9149	DELTA-C	Calculated
1306	CONDUA.BLK.LMTD	11.3575	DELTA-C	Calculated
1309	CONDUA.BLK.FTU	30000	KCAL/HR-SQM-	Calculated
1310	CONDUA.BLK.AREA	40.5678	SQM	Calculated
1311	CONDUA.BLK.QHOT_HEAT	13.8226	MMKCAL/HR	Calculated
1312	CIN.BLK.MASS	133845	KG/HR	Calculated

4 Go to the **Blocks | CONDUA | Results | Convective** sheet to examine the results listed in another format.



5 Go to the **Results Summary | Streams | Material** sheet to examine flow rates and temperatures.



	B	CIN	COUT	D	F
Temperature C	-5.2	-38.5	-40.1	-29.2	25.0
Pressure bar	21.500	1.500	1.400	20.000	25.000
Vapor Frac	0.000	0.000	1.000	0.000	1.000
Mole Flow kmol/hr	356.617	3180.673	3180.673	1400.393	1757.041
Mass Flow kg/hr	10712.573	133844.777	133844.777	39286.569	50000.000
Volume Flow cum/hr	28.051	221.754	42313.678	95.389	1448.677
Enthalpy MMkcal/hr	-8.070	-1.935	11.887	13.242	10.032
Mass Flow kg/hr					
C2H4	150.067			39282.358	39433.283
C2H6	10562.506			4.211	10566.717
C3H6		133844.777	133844.777		
Mole Flow kmol/hr					
C2H4	5.349			1400.253	1405.633
C2H6	351.268			0.140	351.408
C3H6		3180.673	3180.673		

6 Save the simulation file.

Running an EO Optimization

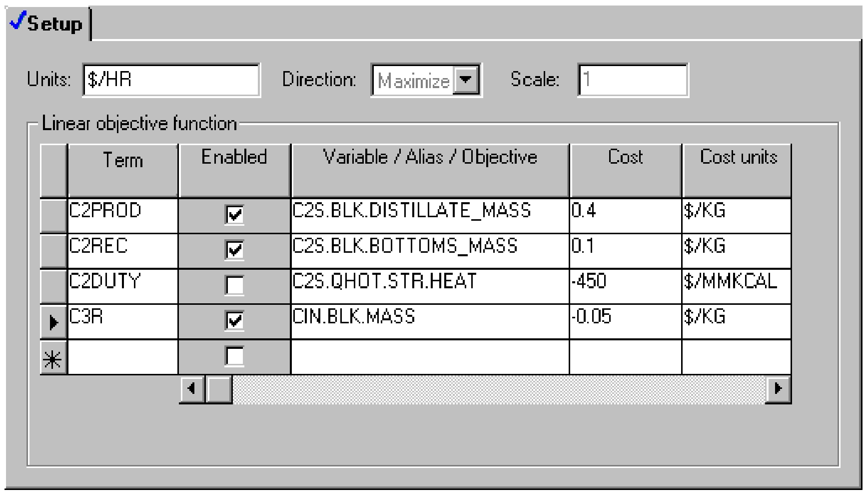
Although it is possible to run an optimization case as the model stands now, it would be more realistic to replace the cost per unit of duty that was entered previously with a cost for the propylene utility stream.

Change the objective function to use propylene cost rather than the estimated cost per MMkcal per hour.

Change the Objective Function

1. Go to the **EO Configuration | Objective | Profit | Input | Setup** sheet.
2. Clear the **Enabled** checkbox for C2DUTY to remove it from the objective function.
3. Add the following term to replace the C2DUTY term:

Term	Variable	Cost	Units
C3R	CIN.BLK.MASS	-0.05	$/KG



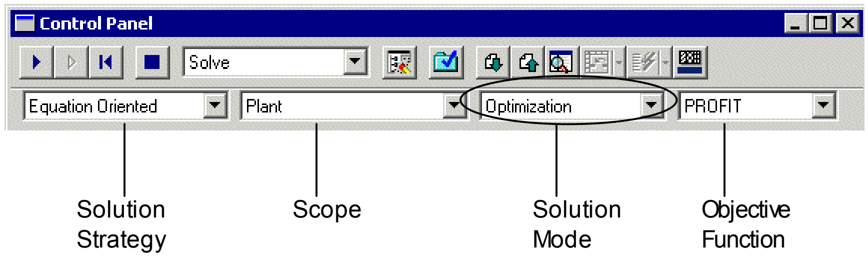
You are now ready to run an EO Optimization of the flowsheet and view the results.

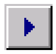
This optimization varies the distillate and bottoms compositions within their specified ranges to achieve an economic optimum based on the given values of the distillate and bottoms mass flows and the cost of the propylene coolant required for the condenser.

Run an EO Optimization Solution

1. Go to the **EO Configuration | Objective** object manager and make sure PROFIT is selected.
2. Go to the **EO Configuration | Spec Groups | Specifications** sheet and make sure the distillate ethane and bottoms ethylene concentration variables are set to Optimized (part of the C2COMPS Spec Group).
3. Go to the **EO Configuration | EO Input | Configure** sheet and make sure there are ranges (upper and lower bounds) entered for your two Optimized variables.
4. Go to the **Control Panel**.
5. In the **Solution mode** field, select **Optimization**.

   The **Objective Function** field should be set to **PROFIT**.



6 Click  to run the optimization.

The solver iterates a few times as it seeks the optimal operating conditions.

Next, examine the results of the optimization run.

View the Optimization Results

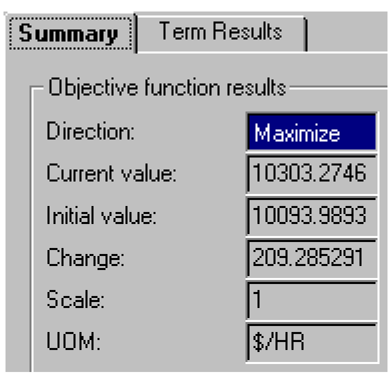
1 Go to the **EO Configuration | EO Variables** form.

2 Double-click the **Specification** column header twice to bring the Optimized and Constant variables to the top.

Index	Variable	Value	Units	Specification	Lower Bound	Upper Bound
14	C2S.D.STR.C2H6	0.0002	FRACTION	Optimized	1e-005	0.0002
20	C2S.B.STR.C2H4	0.00784936	FRACTION	Optimized	0.001	0.05

As in the first optimization, the distillate ethane composition is at its upper bound. However, the bottoms ethylene composition is now higher.

3 Go to the **EO Configuration | Objective | PROFIT | Results | Summary** sheet to examine the new profit value based on the cost of propylene.



4 Save the simulation file.

5 Exit from Aspen Plus.

Note: This simulation is delivered as backup file, **eogsg2**, in the Aspen Plus Examples Library. Use this backup file to check your results.

3 Parameter Estimation

This session utilizes the measurement model to perform a parameter estimation to tune a process flowsheet to plant data.

You will:

- Add a Measurement block to the Process Flowsheet and define Measurement model variables.
- Run the optimization from the previous chapter with the Measurement model in place.
- Perform a parameter estimation to determine the Murphree efficiency and feed stream specifications based on sample plant measurements.
- Perform an economic optimization using the results of the parameter estimation.

Allow about 45 minutes to do this simulation.

Overview of Parameter Estimation

Assume there are plant measurements for the following quantities in our sample flowsheet:

- Feed mass flow
- Feed ethane mole fraction
- Distillate mass flow
- Distillate ethane mole fraction
- Bottoms mass flow
- Bottoms ethylene mole fraction
- Mass reflux ratio
- Propylene stream mass flow

Five of these measurements will be used to define operating conditions. Their values will be imposed on the model and thus have zero offset. The model will predict all the other quantities. The five key measurements are:

- Distillate mass flow
- Distillate ethane mole fraction
- Bottoms mass flow
- Bottoms ethylene mole fraction
- Mass reflux ratio

The parameter estimation run will then determine the following:

- Offset for the feed mass flow
- Offset for the feed ethane mole fraction
- Offset for the propylene stream mass flow
- Tower Murphree efficiency

The term *offset* above refers to the difference between the plant measurement and the model prediction.

Understanding Measurements

Measurements are a convenient way of using process data in a model calculation. You can use measurements in either Sequential Modular (SM) or Equation Oriented (EO) strategy.

A Measurement block consists of one or more measurements. Each measurement is connected to an EO (open) variable, an SM (closed) variable, or both. If no closed variable is entered, the measurement will not affect the SM simulation; if no open variable is entered, the measurement will be created but unconnected to the EO simulation.

In the EO strategy, the Measurement model provides three variables and one equation/residual for each measurement. The variables are:

- Plant
- Model
- Offset

The Plant variable is the actual value of the measurement. The Model variable is the predicted value of the measurement. The Offset variable is the difference between the Plant and the Model variables.

The following equation relates these three quantities in SM strategy:

offset = plant – model

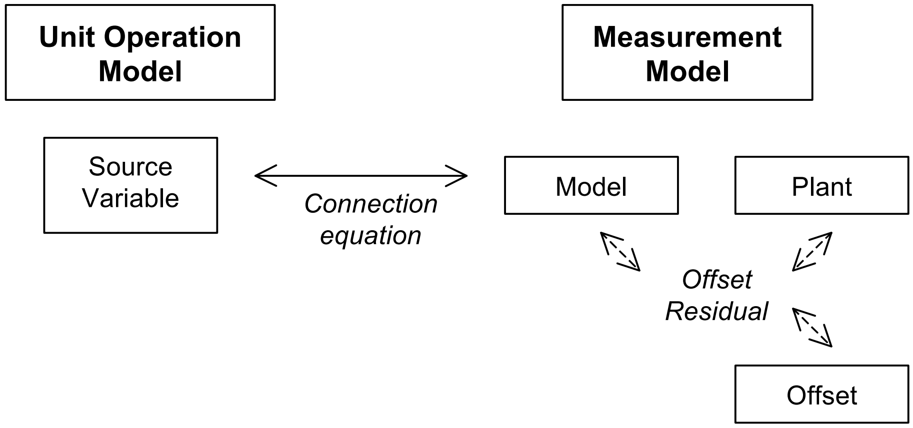
In EO strategy, the equivalent residual (*r*) is:

r = plant – model – offset

In addition, a connection equation relates the measurement model to the specified open variable, called the Source variable. The Measurement model performs this connection automatically. As a result, the Model variable has the same value as the Source variable at the EO solution.

The plant variable is supplied with an initial value by the user or Aspen OnLine.

The following figure illustrates the relationship between the unit operation model and the measurement model.



Source variable, Model variable, Plant variable and Offset variable.

To set up a measurement, you add a Measurement block to the flowsheet and configure the block. Measurement processing automatically creates the three EO variables, using the following naming format:

blockid*.BLK.*tag_description_variable

Where:

- ***blockid*** is the name of the measurement block.
- ***tag*** is the tag specified for each measurement.
- ***description*** is the description provided for each measurement.
- ***variable*** is PLANT, MODEL, or OFFSET.

If the description is not provided, the variables have shorter names in the form ***blockid*.BLK.*tag_variable***.

Calculating Measurements

The **Calculate** option on the **Input | Measurements** sheet defines how the specifications of the measurement variables are set. The options and their effects on the variable specifications are:

Before connection processing

Calculation Option	Variable Specifications			
	Source	**Model**	**Plant**	**Offset**
Calc-Model	Constant	Calculated	Constant	Constant
Calc-Offset*	Calculated	Constant	Constant	Calculated
Calc-Plant	Calculated	Constant	Calculated	Constant
Param-Offset	Calculated	Constant	Measured	Parameterized

After connection processing

Calculation Option	Variable Specifications			
	Source	**Model**	**Plant**	**Offset**
Calc-Model	Calculated	Calculated	Constant	Constant
Calc-Offset*	Calculated	Calculated	Constant	Calculated
Calc-Plant	Calculated	Calculated	Calculated	Constant
Param-Offset	Calculated	Calculated	Measured	Parameterized

*Calc-Offset is the default.

Note that the Calc-Model option should only be used with a source variable that is initially Constant, and is limited to one measurement per Measurement block.

When the measurement connection is processed, the model variable is taken as the connection Destination variable. Normal rules for the specification management of connections are applied and the net specification of the problem is preserved.

For example, consider a case where Calc-Offset is chosen for a measurement block and the Source variable is Calculated. After measurement processing, the Source, Model, and Offset variables are Calculated and the Plant variable is Constant.

Typical Measurement Specifications

You can use Spec Groups to change the specifications of the measurement variables to other combinations. A convenient way to understand these specification combinations is the Measurement Specification.

A Measurement Specification is a combination of the Plant and Offset variable specifications, as listed in the table below.

Table 3.1: Definitions of Measurement Specifications

Measurement Specification	Plant Variable Specification	Offset Variable Specification
Calculated	Measured	Parameterized
Constant	Constant	Constant
Measured	Measured	Constant
Parameterized	Constant	Parameterized
Optimized	Optimized	Constant
Reconciled	Constant	Reconciled
Independent	Optimized	Reconciled

When you want to set a specification on a variable which is the source variable of a measurement, do not change the specification of the source variable. Instead, set the Plant and Offset variables to the combination of specifications corresponding to that Measurement Specification.

Thus, if you want to set a flow rate to Parameterized, and you have a measurement attached to that flow rate, set the Plant variable specification in the measurement to Constant and the Offset variable specification to Parameterized.

Adding a Measurement Block

Add a Measurement block to the Process Flowsheet. Configure the block by specifying which unit operation model variables are connected to the Measurement model. Also, define a Tag for each variable. Each Tag should be a name for its variable that is easy to remember.

For each specified variable, the Measurement model will create three additional EO variables: a Plant variable, a Model variable, and an Offset variable.

The complete set of EO variables (called Open variables) will consist of unit operation model variables and Measurement model variables.

1 Open the simulation file from the previous chapter, **EO2apw**.

2 Save the simulation as **EO3apw**.

3 Open the **Data Browser** (click or press **F8**).

4 Go to the **Flowsheeting Options | Measurement** object manager.

5 Click **New** to create a new Measurement block.

The **Create New ID** dialog box appears.

6 Type **C2MEAS** and click **OK**.

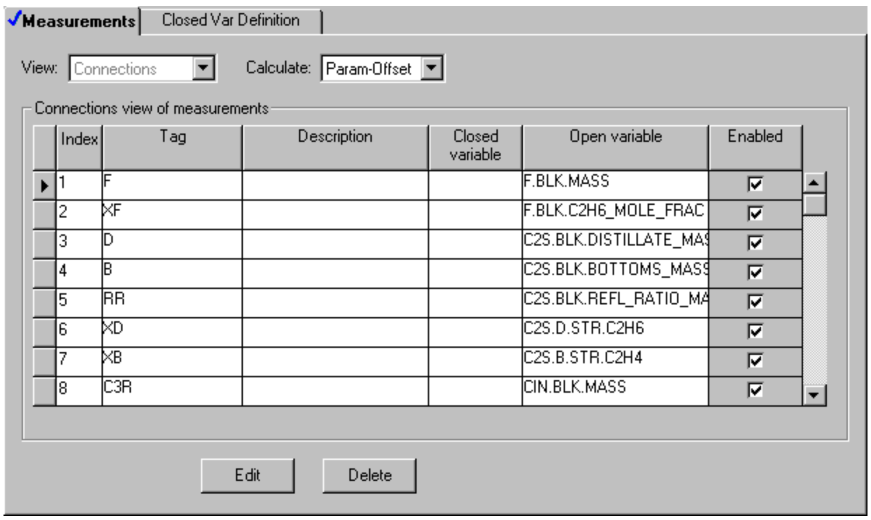
The **Flowsheeting Options | Measurement | C2MEAS | Input | Measurements** sheet appears.

7 In the **View** field, make sure **Connections** is selected.

8 In the **Calculate** field, select **Param-Offset**.

9 Specify eight unit operation model Open variables and their Tags according to the following table:

Index	Tag	Open Variable
1	F	F.BLK.MASS
2	XF	F.BLK.C2H6_MOLE_FRAC
3	D	C2S.BLK.DISTILLATE_MASS
4	B	C2S.BLK.BOTTOMS_MASS
5	RR	C2S.BLK.REFL_RATIO_MASS
6	XD	C2S.D.STR.C2H6
7	XB	C2S.B.STR.C2H4
8	C3R	CIN.BLK.MASS

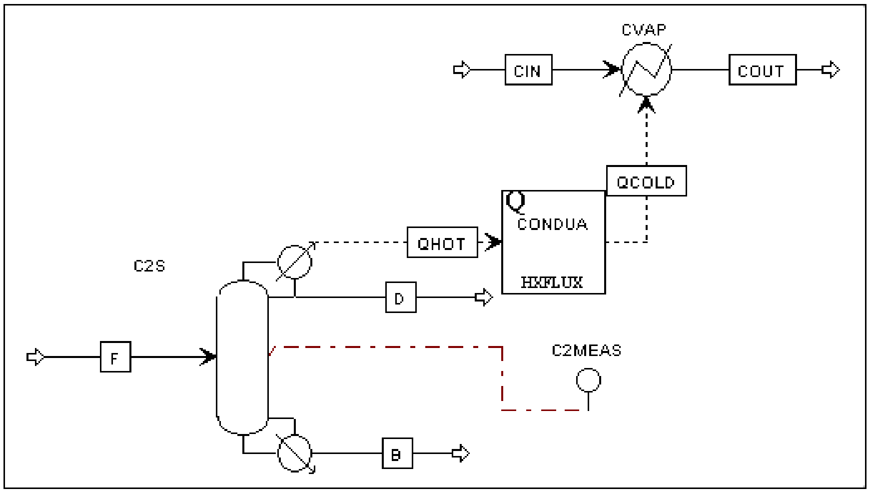


The unit operation model Open variables specified above act as Source variables for the Measurement model. The Source variable and the Model variable are connected together and always have the same value at the solution.

In this session, no unit operation model Closed variables are specified. Specification of Closed variables connects the SM solution to the Measurement model. Since no Closed variables are specified, the SM solution will not use the Measurement model to determine flowsheet operating conditions.

10 Go to the Process Flowsheet to verify that the Measurement block (**C2MEAS**) has been placed. If it does not appear, choose **Tools | Options | Flowsheet** (tab) and select the **Display measurements** checkbox with the **All Blocks and Connections** option chosen. You may also want to turn off **Display connections streams** since they can get in the way. Click **OK**.

The Process Flowsheet with the Measurement block added looks like this:



The measurement connection between the C2MEAS block and the C2S block appears as a red dashed line.

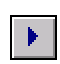
Specifying Measurement Variables

For the first parameter estimation, we wish to run the same basic specifications as before. So, the measurements will be specified as follows:

Measurement	Specification
F	Constant
XF	Constant
XD	Optimized
XB	Optimized
D	Calculated
B	Calculated
RR	Calculated
C3R	Calculated

When the measurement block was set up, we chose a Calculate option of Param-Offset. This means the measurement specification is Calculated. Thus, a Calculate option of Param-Offset will correctly set up measurements D, B, RR and C3R. The other measurements, F, XF, XD and XB will have to be changed in a Spec Group to the proper specification.

Moreover, the Param-Offset option implicitly assumes that the Source variables are Calculated. If not, the measurement will not be built correctly. We can verify this by performing an EO synchronization.

Open the **Control Panel** and click . When Aspen Plus performs an EO synchronization, you will see the following messages generated because some source variables are not Calculated:

```
->Starting EO Synchronization ...

All blocks were placed successfully
The specifications for these measurements are not as expected:
Measurement -Connected?- -Model- -Source-
C2MEAS.XB       Yes       Calc    Optim
C2MEAS.XD       Yes       Calc    Optim
C2MEAS.XF       Yes       Calc    Const
C2MEAS.F        Yes       Calc    Const

->Finished EO Synchronization ...
```

The Model variables are shown as Calculated in the errors because this is the result of connection processing. Normally, there should be one Free and one Fixed variable in a Model-Source pair before connection processing and both should be Calculated at the end of connection processing.

In order to remove these errors, we must change the specifications of the Model variables to Calculated. Again, this can be done in a Spec Group. Remember that Spec Groups are processed before Connections.

When a variable appears in more than one Spec Group, the last specification applied overrides any earlier specifications. Spec Groups within specific blocks are applied before global Spec Groups; Spec Groups on the same form are applied in the order they appear.

Note: It is also possible to disable the C2COMPS Spec Group and re-enter the specifications you want to keep. To disable a Spec Group, clear its **Enabled** checkbox on the Spec Groups form.

Specify Plant, Offset, and Source Variables

1 Go to the **EO Configuration | Spec Groups | Specifications** sheet.

2 In the first blank row in the **Spec group** column, type **TYPSPEC** and press **Enter** on the keyboard

3 Select the **TYPSPEC** row and click **Edit**.

The **Define Spec Groups** dialog box appears.

4 In the **Description** field enter *Typical measurement model spec group*.

In this Spec Group, you need to set specifications on Plant and Offset variables to match the previous table of measurement specifications. You also need to set the Model variables to Calculated to override the previous Spec Group.

The specifications for Calculated variables B, D, RR, and C3R are already set properly.

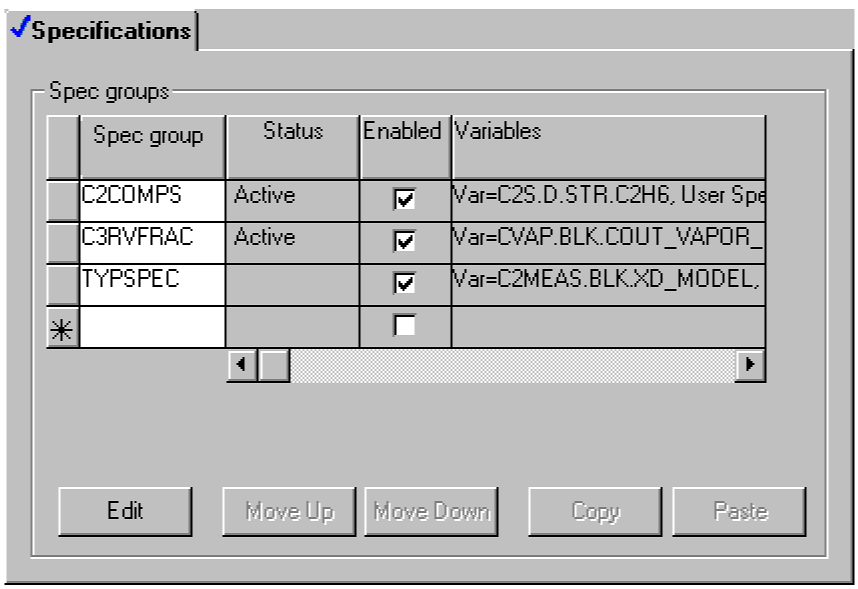
For the EO Simulation run, F and XF will be kept Constant at the measured value. Set these two Model variables to Calculated so that the Source variables will be determined by the measured values.

5 Enter the following **Variables** and **User specs**:

Variable	User Spec
C2MEAS.BLK.XD_MODEL	Calculated
C2MEAS.BLK.XD_PLANT	Optimized
C2MEAS.BLK.XD_OFFSET	Constant
C2MEAS.BLK.XB_MODEL	Calculated
C2MEAS.BLK.XB_PLANT	Optimized
C2MEAS.BLK.XB_OFFSET	Constant
C2MEAS.BLK.F_MODEL	Calculated
C2MEAS.BLK.F_PLANT	Constant
C2MEAS.BLK.F_OFFSET	Constant
C2MEAS.BLK.XF_MODEL	Calculated
C2MEAS.BLK.XF_PLANT	Constant
C2MEAS.BLK.XF_OFFSET	Constant

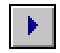
6 Click **Close**.

The **EO Configuration | Spec Groups | Specifications** sheet reappears:



You have added a Measurement model to your Process Flowsheet, defined a set of Tags to create Measurement variables, specified the Plant and Offset variables appropriately, and specified all the Source variables as Calculated.

Checking Variable Specifications

Open the **Control Panel** and click . When Aspen Plus performs an EO synchronization, now there will not be any errors.

Since we are using measurements to drive the flowsheet, we must enter values for all Plant variables in an EO Input form. Moreover, we should remove the values and bounds for the top and bottoms compositions and instead apply these attributes to the Plant variables.

Use the **EO Input** form to set the Plant variables.

Set Values and Bounds for Plant Variables

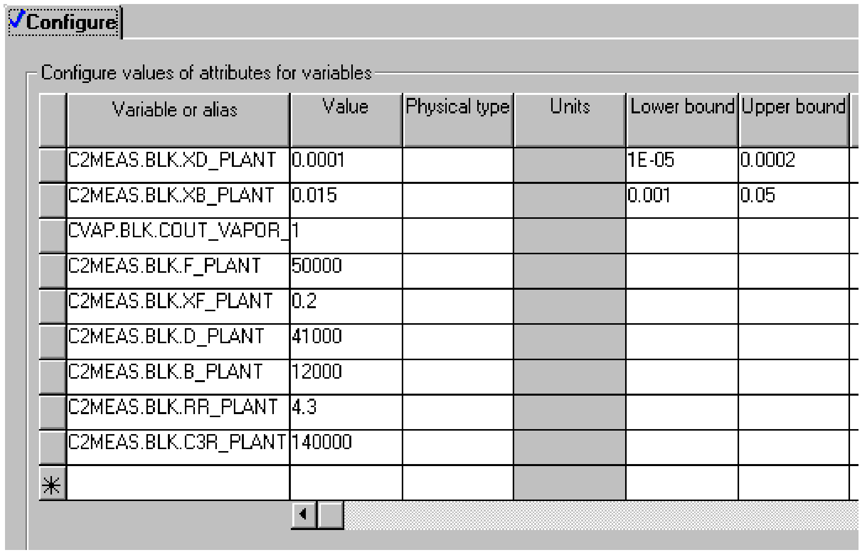
1 Go to the **EO Configuration | EO Input | Configure** sheet.

2 In the **Variable or alias** column, change the XD and XB Source variables to the corresponding Measurement model Plant variables.

Change this	To this
C2S.D.STR.C2H6	C2MEAS.BLK.XD_PLANT
C2S.B.STR.C2H4	C2MEAS.BLK.XB_PLANT

3 In the next available blank rows in the **Variable or alias** column enter the other plant variables. In the corresponding rows in the **Value** column, enter the following plant data:

Variable or alias	Value
C2MEAS.BLK.F_PLANT	50000
C2MEAS.BLK.XF_PLANT	0.2
C2MEAS.BLK.D_PLANT	41000
C2MEAS.BLK.B_PLANT	12000
C2MEAS.BLK.RR_PLANT	4.3
C2MEAS.BLK.C3R_PLANT	140000



Configure

Configure values of attributes for variables

Variable or alias	Value	Physical type	Units	Lower bound	Upper bound
C2MEAS.BLK.XD_PLANT	0.0001			1E-05	0.0002
C2MEAS.BLK.XB_PLANT	0.015			0.001	0.05
CVAP.BLK.COUT_VAPOR_	1				
C2MEAS.BLK.F_PLANT	50000				
C2MEAS.BLK.XF_PLANT	0.2				
C2MEAS.BLK.D_PLANT	41000				
C2MEAS.BLK.B_PLANT	12000				
C2MEAS.BLK.RR_PLANT	4.3				
C2MEAS.BLK.C3R_PLANT	140000				

Now the Source variables used in an EO run will be set to the correct values. The lower and upper bounds for the purities (XB and XD) are used only when you set the Solution Mode to Optimization or Reconciliation and specify an Objective Function.

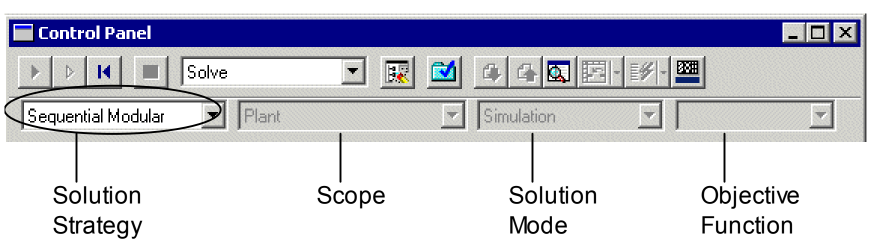
Checking the Spec Group

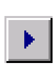
1. For each Plant and each Offset variable in the **TYPSPEC** Spec Group, determine whether it will be Free or Fixed during a Simulation run.
2. For cases where both the Plant and the Offset are Fixed, the Source variable will be determined by the Measurement block. Make sure that it will have the correct value.

   In this example, you specified Plant values for F, XF, XD, and XB, so the Source variables will be set correctly.

Running the Simulation

1. Go to the **Control Panel**.
2. In the **Solution Strategy** field, select **Sequential Modular**.



3. Press **Shift-F5** and click **OK** twice to reinitialize the simulation.
4. Click  to run the simulation. Verify that the SM run converges.
5. In the **Solution Strategy** field, select **Equation Oriented**.

6 Go to the **EO Configuration | EO Variables** form

7 Scroll to the bottom of the list to examine the Measurement block variables.

Index	Variable	Value	Units	Specification
1388	C2MEAS.BLK.F_PLANT	50000	KG/HR	Constant
1389	C2MEAS.BLK.F_MODEL	50000	KG/HR	Calculated
1390	C2MEAS.BLK.F_OFFSET	0	KG/HR	Constant
1391	C2MEAS.BLK.XF_PLANT	0.2	FRACTION	Constant
1392	C2MEAS.BLK.XF_MODEL	0.2	FRACTION	Calculated
1393	C2MEAS.BLK.XF_OFFSET	0	FRACTION	Constant
1394	C2MEAS.BLK.D_PLANT	41000	KG/HR	Measured
1395	C2MEAS.BLK.D_MODEL	39000.5	KG/HR	Calculated
1396	C2MEAS.BLK.D_OFFSET	0	KG/HR	Parameterized
1397	C2MEAS.BLK.B_PLANT	12000	KG/HR	Measured
1398	C2MEAS.BLK.B_MODEL	11000	KG/HR	Calculated
1399	C2MEAS.BLK.B_OFFSET	0	KG/HR	Parameterized
1400	C2MEAS.BLK.RR_PLANT	4.3	UNITLESS	Measured
1401	C2MEAS.BLK.RR_MODEL	3.99995	UNITLESS	Calculated
1402	C2MEAS.BLK.RR_OFFSET	0	UNITLESS	Parameterized
1403	C2MEAS.BLK.XD_PLANT	0.0001	FRACTION	Optimized
1404	C2MEAS.BLK.XD_MODEL	1.65832e-005	FRACTION	Calculated
1405	C2MEAS.BLK.XD_OFFSET	0	FRACTION	Constant
1406	C2MEAS.BLK.XB_PLANT	0.015	FRACTION	Optimized
1407	C2MEAS.BLK.XB_MODEL	0.0421678	FRACTION	Calculated
1408	C2MEAS.BLK.XB_OFFSET	0	FRACTION	Constant
1409	C2MEAS.BLK.C3R_PLANT	140000	KG/HR	Measured
1410	C2MEAS.BLK.C3R_MODEL	150000	KG/HR	Calculated
1411	C2MEAS.BLK.C3R_OFFSET	0	KG/HR	Parameterized

All the Offset variables are initialized to zero. The Model variables are initialized to values from the SM run. The Plant variables are initialized to values on the **EO Input** form. When you run the EO Parameter Estimation, the Plant variables for all the measurements will be fixed to the specified values.

8 Set the **Solution Mode** to Parameter Estimation.

9 Run the problem.

10 Go to the **EO Configuration | EO Variables** form to examine the post-run Measurement block variables.

Index	Variable	Value	Units	Specification
1388	C2MEAS.BLK.F_PLANT	50000	KG/HR	Constant
1389	C2MEAS.BLK.F_MODEL	50000	KG/HR	Calculated
1390	C2MEAS.BLK.F_OFFSET	0	KG/HR	Constant
1391	C2MEAS.BLK.XF_PLANT	0.2	FRACTION	Constant
1392	C2MEAS.BLK.XF_MODEL	0.2	FRACTION	Calculated
1393	C2MEAS.BLK.XF_OFFSET	0	FRACTION	Constant
1394	C2MEAS.BLK.D_PLANT	41000	KG/HR	Measured
1395	C2MEAS.BLK.D_MODEL	39287.4	KG/HR	Calculated
1396	C2MEAS.BLK.D_OFFSET	1712.57	KG/HR	Parameterized
1397	C2MEAS.BLK.B_PLANT	12000	KG/HR	Measured
1398	C2MEAS.BLK.B_MODEL	10712.6	KG/HR	Calculated
1399	C2MEAS.BLK.B_OFFSET	1287.43	KG/HR	Parameterized
1400	C2MEAS.BLK.RR_PLANT	4.3	UNITLESS	Measured
1401	C2MEAS.BLK.RR_MODEL	3.51281	UNITLESS	Calculated
1402	C2MEAS.BLK.RR_OFFSET	0.787186	UNITLESS	Parameterized
1403	C2MEAS.BLK.XD_PLANT	0.0001	FRACTION	Optimized
1404	C2MEAS.BLK.XD_MODEL	0.0001	FRACTION	Calculated
1405	C2MEAS.BLK.XD_OFFSET	0	FRACTION	Constant
1406	C2MEAS.BLK.XB_PLANT	0.015	FRACTION	Optimized
1407	C2MEAS.BLK.XB_MODEL	0.015	FRACTION	Calculated
1408	C2MEAS.BLK.XB_OFFSET	0	FRACTION	Constant
1409	C2MEAS.BLK.C3R_PLANT	140000	KG/HR	Measured
1410	C2MEAS.BLK.C3R_MODEL	133845	KG/HR	Calculated
1411	C2MEAS.BLK.C3R_OFFSET	6154.86	KG/HR	Parameterized

For this simple Parameter Estimation, the Offsets for the four key measurements, F, XF, XD and XB, are zero. The remaining offsets indicate the degree of plant-model mismatch.

11 Save the simulation.

Setting Up a Parameter Estimation

In this next case, a more complex Parameter Estimation will be set up. Here we will use the following measurement specifications:

Measurement	Specification
F	Parameterized
XF	Parameterized
XD	Optimized
XB	Optimized
D	Measured
B	Measured
RR	Measured
C3R	Calculated

Additionally, the column Murphree efficiency will be Parameterized.

These specifications will allow the Parameter Estimation to update the feed flow and composition as well as the column Murphree Efficiency. The offsets for five of the measurements, XD, XB, D, B and RR, will be zero.

The net specification of the problem is unchanged.

Rather than editing the Spec Group **TYPSPEC**, create a separate Spec Group containing the new specifications necessary for this run. This way you can easily return to the previous set of specifications by disabling the new Spec Group. Add this at the end of the list of Spec Groups so that it will override earlier Spec Groups.

Setting up the Parameter Estimation consists of the following steps:

- Set the measurement variables for D, B, and RR to a Measurement Specification of Measured.
- Set the measurement variables for F and XF to a Measurement Specification of Parameterized.
- Set the Murphree efficiency (C2S.BLK.EFF_1) specification to Parameterized.
- Check your Spec Group to verify that the specifications are sensible.

Specify Plant, Offset, and Source Variables

1 Go to the **EO Configuration | Spec Groups | Specifications** sheet.

2 In the first available blank row in the **Spec group** column, type **PARSPEC** and press **Enter** on the keyboard

3 Select the **PARSPEC** row and click **Edit**.

The **Define Spec Groups** dialog box appears.

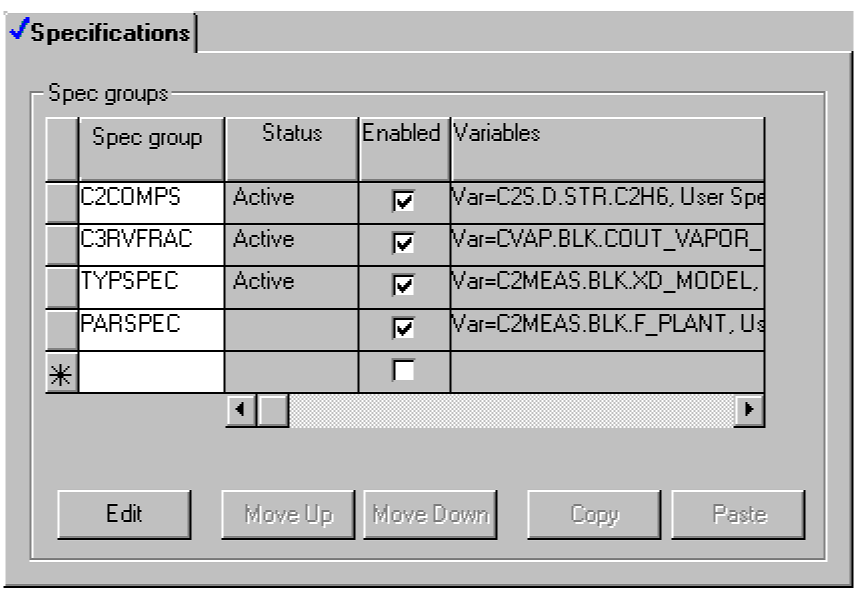
4 In the **Description** field enter *Specifications for parameter estimation*.

5 Enter the following variables and user specs:

Variable	User Spec
C2MEAS.BLK.F_PLANT	Constant
C2MEAS.BLK.F_OFFSET	Parameterized
C2MEAS.BLK.XF_PLANT	Constant
C2MEAS.BLK.XF_OFFSET	Parameterized
C2MEAS.BLK.D_PLANT	Measured
C2MEAS.BLK.D_OFFSET	Constant
C2MEAS.BLK.B_PLANT	Measured
C2MEAS.BLK.B_OFFSET	Constant
C2MEAS.BLK.RR_PLANT	Measured
C2MEAS.BLK.RR_OFFSET	Constant
C2S.BLK.EFF_1	Parameterized

6 Click **Close**.

The EO Configuration | Spec Groups | Specifications sheet reappears:



Check the Specifications

Open the **Control Panel**. In the **Command Line** at the bottom, enter the command:

check measurements

Press **Enter** on the keyboard. In the message area of the **Control Panel**, Aspen Plus should respond that *All measurements are correctly specified*.

Running the Parameter Estimation

1 Go to the **Control Panel**.

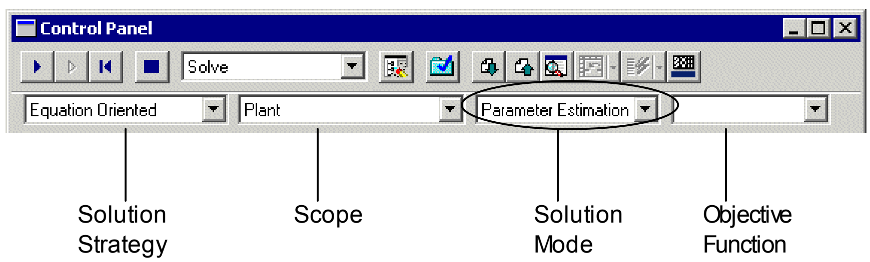
2 In the **Solution Strategy** field, select **Sequential Modular**.

3 Press Shift-F5 and click **OK** twice to reinitialize the simulation.

4 Run the simulation.

5 In the **Solution Strategy** field, select **Equation Oriented**.

6 In the **Solution Mode** field, select **Parameter Estimation**.



7 Run the problem.

8 Go to the **EO Configuration | EO Variables** form.

9 Scroll to the bottom of the list to examine the Measurement block variables.

Index	Variable	Value	Units	Specification
1388	C2MEAS.BLK.F_PLANT	50000	KG/HR	Constant
1389	C2MEAS.BLK.F_MODEL	53000	KG/HR	Calculated
1390	C2MEAS.BLK.F_OFFSET	-3000	KG/HR	Parameterized
1391	C2MEAS.BLK.XF_PLANT	0.2	FRACTION	Constant
1392	C2MEAS.BLK.XF_MODEL	0.214612	FRACTION	Calculated
1393	C2MEAS.BLK.XF_OFFSET	-0.014612	FRACTION	Parameterized
1394	C2MEAS.BLK.D_PLANT	41000	KG/HR	Measured
1395	C2MEAS.BLK.D_MODEL	41000	KG/HR	Calculated
1396	C2MEAS.BLK.D_OFFSET	0	KG/HR	Constant
1397	C2MEAS.BLK.B_PLANT	12000	KG/HR	Measured
1398	C2MEAS.BLK.B_MODEL	12000	KG/HR	Calculated
1399	C2MEAS.BLK.B_OFFSET	0	KG/HR	Constant
1400	C2MEAS.BLK.RR_PLANT	4.3	UNITLESS	Measured
1401	C2MEAS.BLK.RR_MODEL	4.3	UNITLESS	Calculated
1402	C2MEAS.BLK.RR_OFFSET	0	UNITLESS	Constant
1403	C2MEAS.BLK.XD_PLANT	0.0001	FRACTION	Optimized
1404	C2MEAS.BLK.XD_MODEL	0.0001	FRACTION	Calculated
1405	C2MEAS.BLK.XD_OFFSET	0	FRACTION	Constant
1406	C2MEAS.BLK.XB_PLANT	0.015	FRACTION	Optimized
1407	C2MEAS.BLK.XB_MODEL	0.015	FRACTION	Calculated
1408	C2MEAS.BLK.XB_OFFSET	0	FRACTION	Constant
1409	C2MEAS.BLK.C3R_PLANT	140000	KG/HR	Measured
1410	C2MEAS.BLK.C3R_MODEL	164039	KG/HR	Calculated
1411	C2MEAS.BLK.C3R_OFFSET	-24039.3	KG/HR	Parameterized

Note that the offsets for the five key measurements, XD, XB, D, B, and RR, are zero. The remaining offsets indicate the degree of plant-model mismatch.

10 Scroll toward the top of the list and locate the variable for efficiency, C2S.BLK.EFF_**1** The value is about 0.69.

Index	Variable	Value	Units	Specification
41	C2S.BLK.EFF_1	0.690559	UNITLESS	Parameterized

11 Go to the **Flowsheeting Options | Measurement | C2MEAS | Results** sheet to examine the Measurement variables another way.

Results

Results

Index	TAG	Description	UOM	Plant	Model	Offset	Status
1	F		KG/HR	50000	53000	-3000	Enabled
2	XF		FRACTION	0.2	0.21461203	-0.0146120	Enabled
3	D		KG/HR	41000	41000	0	Enabled
4	B		KG/HR	12000	12000	0	Enabled
5	RR		UNITLESS	4.3	4.3	0	Enabled
6	XD		FRACTION	0.0001	0.0001	0	Enabled
7	XB		FRACTION	0.015	0.015	0	Enabled
8	C3R		KG/HR	140000	164039.349	-24039.349	Enabled

12 Save the simulation.

Running in Optimization Mode

You can change the **Solution Mode** to **Optimization** and immediately run an optimization using the results of the Parameter Estimation.

Switching from Parameter Estimation to Optimization causes variables specified as Measured to switch from Fixed to Free. This means D, RR, and B plant values will be calculated. Variables specified as Parameterized switch from Free to Fixed. This means F and XF plant values, and efficiency will be Fixed, and their values determined in the Parameter Estimation are used for the Optimization run. All offsets will be fixed during the Optimization.

Before running the Optimization, verify that the new meanings of the specifications lead to a sensible EO setup.

Check the Specifications

1 In the **Control Panel**, change the **Solution Mode** to Optimization

2 In the **Command Line**, enter the command:

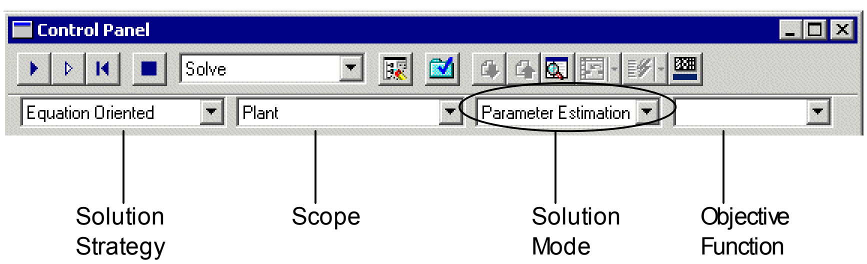
check measurements

Aspen Plus should indicate that all measurements are correctly specified.

Now you are ready to run the EO Optimization using the same Spec Groups as were used in the Parameter Estimation. The Murphree efficiency and the Feed stream flow rate and composition obtained in the Parameter Estimation will automatically be used in the Optimization.

Run the EO Optimization

1 In the **Control Panel**, select PROFIT for the **Objective Function**.



2 Run the optimization.

3 Go to the **EO Configuration | EO Variables** sheet.

4 Scroll to the bottom of the sheet to examine the Measurement block variables.

Index	Variable	Value	Units	Specification
1388	C2MEAS.BLK.F_PLANT	50000	KG/HR	Constant
1389	C2MEAS.BLK.F_MODEL	53000	KG/HR	Calculated
1390	C2MEAS.BLK.F_OFFSET	-3000	KG/HR	Parameterized
1391	C2MEAS.BLK.XF_PLANT	0.2	FRACTION	Constant
1392	C2MEAS.BLK.XF_MODEL	0.214612	FRACTION	Calculated
1393	C2MEAS.BLK.XF_OFFSET	-0.014612	FRACTION	Parameterized
1394	C2MEAS.BLK.D_PLANT	40885.6	KG/HR	Measured
1395	C2MEAS.BLK.D_MODEL	40885.6	KG/HR	Calculated
1396	C2MEAS.BLK.D_OFFSET	0	KG/HR	Constant
1397	C2MEAS.BLK.B_PLANT	12114.4	KG/HR	Measured
1398	C2MEAS.BLK.B_MODEL	12114.4	KG/HR	Calculated
1399	C2MEAS.BLK.B_OFFSET	0	KG/HR	Constant
1400	C2MEAS.BLK.RR_PLANT	3.97972	UNITLESS	Measured
1401	C2MEAS.BLK.RR_MODEL	3.97972	UNITLESS	Calculated
1402	C2MEAS.BLK.RR_OFFSET	0	UNITLESS	Constant
1403	C2MEAS.BLK.XD_PLANT	0.0002	FRACTION	Optimized
1404	C2MEAS.BLK.XD_MODEL	0.0002	FRACTION	Calculated
1405	C2MEAS.BLK.XD_OFFSET	0	FRACTION	Constant
1406	C2MEAS.BLK.XB_PLANT	0.0253416	FRACTION	Optimized
1407	C2MEAS.BLK.XB_MODEL	0.0253416	FRACTION	Calculated
1408	C2MEAS.BLK.XB_OFFSET	0	FRACTION	Constant
1409	C2MEAS.BLK.C3R_PLANT	129658	KG/HR	Measured
1410	C2MEAS.BLK.C3R_MODEL	153697	KG/HR	Calculated
1411	C2MEAS.BLK.C3R_OFFSET	-24039.3	KG/HR	Parameterized

The F and XF Model (and therefore Source) variables were set according to the results of the previous run using the fixed value from the **EO Input** form and the Offset from the previous run.

5 Save the simulation

6 Exit Aspen Plus.

Note: This simulation is delivered as backup file, **eogsg3**, in the Aspen Plus Examples Library. Use this backup file to check your results.

4 Reconciliation

This session utilizes the measurement model to perform a reconciliation to tune the model to plant data. This is an optimization function, which gives different results than the parameter estimation.

You will:

- Define a sum of squares objective function
- Perform a reconciliation
- Perform an economic optimization at the model tuned point

Allow about 45 minutes to do this simulation.

Overview of Reconciliation

As before, there are plant measurements for the following items:

- Feed mass flow
- Feed ethane mole fraction
- Distillate mass flow
- Distillate ethane mole fraction
- Bottoms mass flow
- Bottoms ethylene mole fraction
- Mass reflux ratio
- Propylene stream mass flow

For the reconciliation, there are five degree-of-freedom variables:

- Feed mass flow
- Feed ethane mole fraction
- Distillate ethane mole fraction
- Bottoms ethylene mole fraction
- Tower Murphree efficiency

The solver will manipulate these degree-of-freedom variables to minimize a sum of squares objective function. The objective function will include all eight of the measurement offsets.

Running an EO Reconciliation

Start this simulation from the previous case.

Starting Aspen Plus From the Previous Run

To start Aspen Plus with the previous run:

1 Start Aspen Plus.

The **Aspen Plus Startup** dialog box appears.

2 From the **Open an Existing Simulation** list, select the simulation file of the previous session, **EO3apw**, or load the backup file **EOGSG3bkp** from the Examples directory.

The flowsheet should appear in the Aspen Plus window.

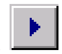
Synchronizing the EO Strategy

You will first solve this simulation with the Sequential Modular (SM) strategy. Then, you will set the strategy to EO to synchronize the model, which creates all the EO variables and simplifies the configuration of the Reconciliation.

1 From the Aspen Plus toolbar, click  to open the **Control Panel**.

2 In the Control Panel, select **Sequential Modular** for the **Solution Strategy**.

3 Press **Shift-F5** and click **OK** twice to reinitialize the simulation.

4 On the Control Panel toolbar, click  to run the simulation.

   As the simulation runs, status messages appear in the Control Panel. Aspen Plus processes input specifications and perform the simulation.

   When the calculations are complete, the message *Results Available* appears in the lower right corner of the Aspen Plus window.

5 In the **Solution Strategy** field, change **Sequential Modular** to **Equation Oriented**.

   When Equation Oriented is selected, the Scope, Mode and Objective fields become active. Changing the solution strategy from SM to EO synchronizes the model.

Changing Measurement Specifications

During the Reconciliation, the Offset variables for the Murphree efficiency, tower product compositions, feed mass flow and composition will be degrees of freedom. These degrees of freedom will be used to minimize the sum of the weighted squares for all of the measurement offsets.

You will make a number of specification changes to perform a Reconciliation. The measurements will have the following specifications:

Measurement	**Specification**
F	Reconciled
XF	Reconciled
XD	Independent
XB	Independent
D	Calculated
B	Calculated
RR	Calculated
C3R	Calculated

F, XF, and the tower efficiency will be Reconciled. XD and XB will also be degrees of freedom for the Reconciliation, but they should remain DOF for Optimizations as well, so they will become Independent. D, B, RR, and C3R will be Calculated.

First, you will disable the PARSPEC Spec Group. Those Measured and Parameterized measurement specifications are not needed for this run. Then use the Measurement Specifications table on page 66 to set the specifications for the Plant and Offset variables.

With the PARSPEC Spec Group disabled, the variables for D, B, RR, and C3R are already in a Calculated measurement specification.

Lastly, the column Murphree efficiency will be Reconciled.

The overall result is that the net specification of the problem is preserved.

1 In the Data Browser tree, expand the **EO Configuration** folder and select **Spec Groups**.

The **EO Configuration | Spec Groups | Specification** sheet appears.

2 In the PARSPEC Spec Group row, clear the Enabled checkbox.

This disables these specification changes.

3 In the first blank line under the **Spec groups** column, enter **RECMODE** and press **Enter** to open a new row in the sheet.

4 Select the **RECMODE** row and click **Edit**.

The **Define Spec Groups** dialog box appears.

5 In the **Description** field, enter *Specifications for reconciliation.*

6 Enter the following variables and user specs:

Variable	User Spec
C2MEAS.BLK.F_PLANT	Constant
C2MEAS.BLK.F_OFFSET	Reconciled
C2MEAS.BLK.XF_PLANT	Constant
C2MEAS.BLK.XF_OFFSET	Reconciled
C2MEAS.BLK.XD_PLANT	Optimized
C2MEAS.BLK.XD_OFFSET	Reconciled
C2MEAS.BLK.XB_PLANT	Optimized
C2MEAS.BLK.XB_OFFSET	Reconciled
C2S.BLK.EFF_1	Reconciled

7 Click **Close** to close the dialog box.

Remember that since Spec Groups are applied in the order in which they appear on the Spec Groups form, these specifications override the previous Spec Groups.

Defining An Objective Function

Next, you will define the sum-of-squares objective function. This includes the offsets of all measurements.

The sum of squares objective function has the following form:

$Objective = \Sigma\, [(\, Offset - Mean\,) / \sigma\,]^2$

Where:

- *Offset* is the measurement offset.
- *Mean* is a mean or average value for the offset, normally zero.
- σ is the standard error of the measurement on an absolute basis.

The larger the standard error, the less weight the measurement has in the objective function and the larger the allowed changes in the reconciled offset.

To specify the objective function:

1 In the Data Browser tree, select the **EO Configuration | Objective** folder.

2 Click **Add** to add a new objective function.

The **Create new ID** dialog box appears.

3 Enter **RECERR** for the ID, and choose the **SUMOFSQUARES** type.

4 Click **OK**.

The **EO Configuration** | **Objective | RECERR | Input | Setup** form appears.

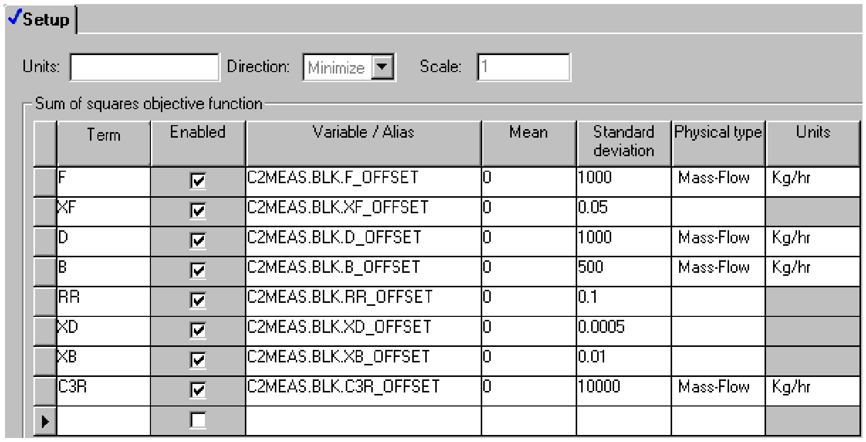
5 Enter the following information. Also enter zero for the **Mean** of each term.

Term	Variable	Standard deviation	Physical type	Units
F	C2MEAS.BLK.F_OFFSET	1000	Mass-Flow	Kg/hr
XF	C2MEAS.BLK.XF_OFFSET	0.05		
D	C2MEAS.BLK.D_OFFSET	1000	Mass-Flow	Kg/hr
B	C2MEAS.BLK.B_OFFSET	500	Mass-Flow	Kg/hr
RR	C2MEAS.BLK.RR_OFFSET	0.1		
XD	C2MEAS.BLK.XD_OFFSET	0.0005		
XB	C2MEAS.BLK.XB_OFFSET	0.01		
C3R	C2MEAS.BLK.C3R_OFFSET	10000	Mass-Flow	Kg/hr

Note: You must enter the **Physical Type** for each variable before specifying the **Units**.

At the top of the sheet, leave the **Units** field blank since this objective function is unitless. The **Direction** defaults to Minimize for sum-of-squares objective functions, which is what we want.

The **EO Configuration | Objective | RECERR | Input | Setup** sheet is complete:



Term	Enabled	Variable / Alias	Mean	Standard deviation	Physical type	Units
F	☑	C2MEAS.BLK.F_OFFSET	0	1000	Mass-Flow	Kg/hr
XF	☑	C2MEAS.BLK.XF_OFFSET	0	0.05		
D	☑	C2MEAS.BLK.D_OFFSET	0	1000	Mass-Flow	Kg/hr
B	☑	C2MEAS.BLK.B_OFFSET	0	500	Mass-Flow	Kg/hr
RR	☑	C2MEAS.BLK.RR_OFFSET	0	0.1		
XD	☑	C2MEAS.BLK.XD_OFFSET	0	0.0005		
XB	☑	C2MEAS.BLK.XB_OFFSET	0	0.01		
C3R	☑	C2MEAS.BLK.C3R_OFFSET	0	10000	Mass-Flow	Kg/hr
	☐					

6 In the Data Browser tree, select to the **Objective** folder.

The **EO Configuration | Objective** object manager appears.

7 In the **Reconciliation** field, select RECERR.

This causes the EO Reconciliation mode to use RECERR as the default objective function.

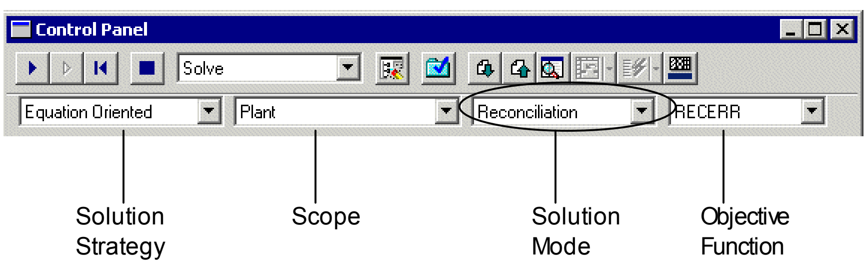
8 Save the simulation as **EO4apw**.

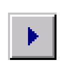
Running the EO Reconciliation

Now run the Equation Oriented (EO) Reconciliation.

To run the EO reconciliation:

1 In the **Control Panel**, select **Reconciliation** for the Solution Mode. RECERR should appear in the Objective Function field. For example:



2 On the Control Panel toolbar, click  to run the EO reconciliation.

This requires several iterations of the solver as it manipulates the five degrees of freedom to minimize the objective function RECERR. If the solver stops because it exceeds the maximum number of iterations, start it again. It will pick up where it left off and converge in a few more iterations.

Viewing the Reconciliation Results

View the results of the EO Reconciliation solution in the EO Variables folder.

To view the EO Reconciliation results:

1 In the Data Browser open the **EO Configuration** | **EO Variables** form.

2 Scroll to the end of the list and locate the variables for block **C2MEAS**.

These are the variables for the measurement model.

Index	Variable	Value	Units	Specification
1388	C2MEAS.BLK.F_PLANT	50000	KG/HR	Constant
1389	C2MEAS.BLK.F_MODEL	51053.7	KG/HR	Calculated
1390	C2MEAS.BLK.F_OFFSET	-1053.73	KG/HR	Reconciled
1391	C2MEAS.BLK.XF_PLANT	0.2	FRACTION	Constant
1392	C2MEAS.BLK.XF_MODEL	0.218009	FRACTION	Calculated
1393	C2MEAS.BLK.XF_OFFSET	-0.0180094	FRACTION	Reconciled
1394	C2MEAS.BLK.D_PLANT	41000	KG/HR	Measured
1395	C2MEAS.BLK.D_MODEL	39350.5	KG/HR	Calculated
1396	C2MEAS.BLK.D_OFFSET	1649.5	KG/HR	Parameterized
1397	C2MEAS.BLK.B_PLANT	12000	KG/HR	Measured
1398	C2MEAS.BLK.B_MODEL	11703.2	KG/HR	Calculated
1399	C2MEAS.BLK.B_OFFSET	296.772	KG/HR	Parameterized
1400	C2MEAS.BLK.RR_PLANT	4.3	UNITLESS	Measured
1401	C2MEAS.BLK.RR_MODEL	4.2524	UNITLESS	Calculated
1402	C2MEAS.BLK.RR_OFFSET	0.0476037	UNITLESS	Parameterized
1403	C2MEAS.BLK.XD_PLANT	0.0001	FRACTION	Optimized
1404	C2MEAS.BLK.XD_MODEL	9.77034e-005	FRACTION	Calculated
1405	C2MEAS.BLK.XD_OFFSET	2.29663e-006	FRACTION	Reconciled
1406	C2MEAS.BLK.XB_PLANT	0.015	FRACTION	Optimized
1407	C2MEAS.BLK.XB_MODEL	0.0151898	FRACTION	Calculated
1408	C2MEAS.BLK.XB_OFFSET	-0.000189836	FRACTION	Reconciled
1409	C2MEAS.BLK.C3R_PLANT	140000	KG/HR	Measured
1410	C2MEAS.BLK.C3R_MODEL	156026	KG/HR	Calculated
1411	C2MEAS.BLK.C3R_OFFSET	-16025.7	KG/HR	Parameterized

3 Review the values for the offsets computed by the parameter estimation.

4 Scroll toward the top of the list and locate the variable for efficiency, C2S.BLK.EFF_1

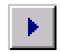
Index	Variable	Value	Units	Specification
41	C2S.BLK.EFF_1	0.703257	UNITLESS	Reconciled

Running an EO Optimization

Now run the Equation-Oriented Optimization problem, using the results of the EO Reconciliation.

To run the EO Optimization solution:

1 In the **Control Panel**, select **Optimization** for the **Solution Mode**. PROFIT should appear in the **Objective** field.

2 On the Control Panel toolbar, click  to run the optimization.

The solver iterates a few times as it seeks the optimum operating conditions.

Viewing the Optimization Results

View the results of the Equation Oriented Optimization solution in the **EO Variables** folder.

To view the EO Optimization results:

1 In the Data Browser tree, expand the **EO Configuration** folder and select **EO Variables**.

The **EO Variables** form appears.

2 Scroll towards the bottom of the list and locate the composition measurement variables C2MEAS.BLK.XD_PLANT and C2MEAS.BLK.XB_PLANT.

1403	C2MEAS.BLK.XD_PLANT	0.0002	FRACTION	Optimized
1404	C2MEAS.BLK.XD_MODEL	0.000197703	FRACTION	Calculated
1405	C2MEAS.BLK.XD_OFFSET	2.29663e-006	FRACTION	Reconciled
1406	C2MEAS.BLK.XB_PLANT	0.0232919	FRACTION	Optimized
1407	C2MEAS.BLK.XB_MODEL	0.0234817	FRACTION	Calculated
1408	C2MEAS.BLK.XB_OFFSET	-0.000189836	FRACTION	Reconciled

These should show the optimized values and have a specification of Optimized.

Since the tower efficiency is slightly higher than the previous example, the optimum bottoms ethylene composition is a little lower.

Exiting Aspen Plus

To exit Aspen Plus:

1 From the **Aspen Plus** menu bar, choose **File | Exit**.

The **Aspen Plus** dialog box appears, asking if you want to save the run.

2 Click **No**.

Note: This simulation is delivered as backup file, **eogsg4**, in the Aspen Plus Examples Library. Use this backup file to check your results.

5 Connecting to the Simulation Engine

After you start the Aspen Plus User Interface, you are prompted for the name of computer running the Aspen Plus simulation engine, if ether of these conditions exist:

- The simulation engine is not installed on your PC.
- The simulation engine is installed on your PC, but the Activator security device is not connected to your PC.

In either of these cases, the **Connect to Engine** dialog box appears.

To connect to the simulation engine:

1 In the **Server type** field, click and select the type of host computer for the simulation engine.

2 If you choose *Local PC* as the server for the simulation engine, you do not need to enter any more information into the dialog box. Click **OK** to continue.

If you choose *Windows 2000 or XP server* as the server for the simulation engine, enter the following additional information:

3 In the Node name field, enter the node name of the computer on which the Aspen Plus simulation engine will execute.

4 In the other fields, enter the following information:

User name	Your user name for the specified host/server.
Password	Your password for the above user name.
Working directory	The associated working directory.

5 Click **OK**.

When the network connection is established, the message Connection Established appears in the dialog box.

If the Connection Established message does not appear, see your Aspen Plus system administrator for more information on network protocols and host computers for the Aspen Plus simulation engine.

General Information

This section provides Copyright details and lists any other documentation related to this release.

Copyright

Version Number: 2004.1

April 2005

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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 Petroleum Processes	Tutorials covering the Aspen Plus features designed to handle petroleum
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 Processes with Electrolytes	Tutorials covering the Aspen Plus features designed to handle electrolytes
Aspen Plus Getting Started Modeling Processes with Solids	Tutorials covering the Aspen Plus features designed to handle solids
Aspen Engineering Suite Installation Manual	Instructions for installing Aspen Plus and other Aspen Engineering Suite products
Aspen Plus User Guide	Procedures for using Aspen Plus

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