Aspen Engineering Suite 2004.1

Aspen Plus 2004.1

Getting Started Using Equation Oriented Modeling
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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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:

<table>
<thead>
<tr>
<th>SM Solution Mode</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simulation</td>
<td>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.</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>EO Solution Mode</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simulation</td>
<td>This mode is a prediction mode and has no degrees of freedom. For given feed conditions and operating parameters, compute the products.</td>
</tr>
<tr>
<td>Parameter Estimation</td>
<td>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.</td>
</tr>
<tr>
<td>Reconciliation</td>
<td>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</td>
</tr>
<tr>
<td>Optimization</td>
<td>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.</td>
</tr>
</tbody>
</table>

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).

<table>
<thead>
<tr>
<th>Status</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fixed</td>
<td>The solver cannot change the variable value. It is a fixed input. You specify its value.</td>
</tr>
<tr>
<td>Free</td>
<td>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.</td>
</tr>
<tr>
<td>Degree of Freedom (DOF)</td>
<td>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.</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Specification</th>
<th>Simulation</th>
<th>Parameter Estimation</th>
<th>Reconciliation</th>
<th>Optimization</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calculated</td>
<td>Free</td>
<td>Free</td>
<td>Free</td>
<td>Free</td>
</tr>
<tr>
<td>Constant</td>
<td>Fixed</td>
<td>Fixed</td>
<td>Fixed</td>
<td>Fixed</td>
</tr>
<tr>
<td>Measured</td>
<td>Free</td>
<td>Fixed</td>
<td>Fixed</td>
<td>Free</td>
</tr>
<tr>
<td>Parameterized</td>
<td>Fixed</td>
<td>Free</td>
<td>Free</td>
<td>Fixed</td>
</tr>
<tr>
<td>Optimized</td>
<td>Fixed</td>
<td>Fixed</td>
<td>Fixed</td>
<td>DOF</td>
</tr>
<tr>
<td>Reconciled</td>
<td>Fixed</td>
<td>Fixed</td>
<td>DOF</td>
<td>Fixed</td>
</tr>
<tr>
<td>Independent</td>
<td>Fixed</td>
<td>Fixed</td>
<td>DOF</td>
<td>DOF</td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>The initial value of the variable. If the variable is free during solution in the selected mode, the solution engine may change the value.</td>
</tr>
<tr>
<td>Lower Bound</td>
<td>The minimum allowable value of the variable.</td>
</tr>
<tr>
<td>Upper Bound</td>
<td>The maximum allowable value of the variable.</td>
</tr>
<tr>
<td>Step Bound</td>
<td>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.</td>
</tr>
<tr>
<td>UOM</td>
<td>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.</td>
</tr>
<tr>
<td>Bound Type</td>
<td>One of the following:</td>
</tr>
<tr>
<td></td>
<td>Hard indicates that the bound will be respected at all times. This is the default.</td>
</tr>
<tr>
<td></td>
<td>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.</td>
</tr>
<tr>
<td></td>
<td>Soft indicates that any violation of the bound is multiplied by the soft bound weight and added to the objective function (penalty function).</td>
</tr>
<tr>
<td>Soft Bound Weight</td>
<td>Weighting factor used when the Bound Type is Soft.</td>
</tr>
</tbody>
</table>

**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
### 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.

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

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**.

3. The Aspen Plus window is now active.

4. From the Aspen Plus menu bar, choose **Tools | Options**. The **Options** dialog box appears.

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

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

7. 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:

<table>
<thead>
<tr>
<th>Stream ID</th>
<th>Stream Type</th>
<th>Port</th>
</tr>
</thead>
<tbody>
<tr>
<td>F</td>
<td>Material</td>
<td>Feed (required)</td>
</tr>
<tr>
<td>D</td>
<td>Material</td>
<td>Liquid Distillate (required if distillate vapor fraction &lt; 1)</td>
</tr>
<tr>
<td>B</td>
<td>Material</td>
<td>Bottoms (required)</td>
</tr>
<tr>
<td>QHOT</td>
<td>Heat</td>
<td>Condenser Heat Stream (optional)</td>
</tr>
</tbody>
</table>

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.

![Screenshot of Data Browser](image)

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:

<table>
<thead>
<tr>
<th>Component ID</th>
<th>Type</th>
<th>Component Name</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2H4</td>
<td>Conventional</td>
<td>Ethylene</td>
<td>C2H4</td>
</tr>
<tr>
<td>C2H6</td>
<td>Conventional</td>
<td>Ethane</td>
<td>C2H6</td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Field</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>25°C</td>
</tr>
<tr>
<td>Pressure</td>
<td>25 bar</td>
</tr>
<tr>
<td>Total Flow</td>
<td>Mass 50000 kg/hr</td>
</tr>
<tr>
<td>Composition</td>
<td>Mole-Frac</td>
</tr>
<tr>
<td>C2H4 mole fraction</td>
<td>0.8</td>
</tr>
<tr>
<td>C2H6 mole fraction</td>
<td>0.2</td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Field</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of stages</td>
<td>100</td>
</tr>
<tr>
<td>Condenser</td>
<td>Total</td>
</tr>
</tbody>
</table>

2. Specify the following Operating specifications:

<table>
<thead>
<tr>
<th>Field</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distillate rate</td>
<td>Mass 39000 kg/hr</td>
</tr>
<tr>
<td>Reflux ratio</td>
<td>Mass 4.0</td>
</tr>
</tbody>
</table>

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**:

<table>
<thead>
<tr>
<th>Column</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stage</td>
<td>60</td>
</tr>
<tr>
<td>Convention</td>
<td>Above-Stage</td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Stage</th>
<th>Pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>20</td>
</tr>
<tr>
<td>2</td>
<td>20.5</td>
</tr>
<tr>
<td>60</td>
<td>21.0</td>
</tr>
<tr>
<td>100</td>
<td>21.5</td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Stage</th>
<th>Efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.9</td>
</tr>
</tbody>
</table>

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.

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

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.

![EO Configuration | EO Variables](image)

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:

<table>
<thead>
<tr>
<th>Variable</th>
<th>User Spec</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2S.D.STR.C2H6</td>
<td>Constant</td>
</tr>
<tr>
<td>C2S.B.STR.C2H4</td>
<td>Constant</td>
</tr>
<tr>
<td>C2S.BLK.DISTILLATE_MASS</td>
<td>Calculated</td>
</tr>
<tr>
<td>C2S.BLK.REFL_RATIO_MASS</td>
<td>Calculated</td>
</tr>
</tbody>
</table>

**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.
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.

<table>
<thead>
<tr>
<th>Index</th>
<th>Variable</th>
<th>Value</th>
<th>Units</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>1233</td>
<td>C2S.BLK.DISTILLATE_MOLE</td>
<td>1390.2</td>
<td>KMOL/HR</td>
<td>Calculated</td>
</tr>
<tr>
<td>1234</td>
<td>C2S.BLK.DISTILLATE_MASS</td>
<td>3900.5</td>
<td>KG/M</td>
<td>Calculated</td>
</tr>
<tr>
<td>1235</td>
<td>C2S.BLK.DISTILLATE_STDV</td>
<td>117.756</td>
<td>CM</td>
<td>Calculated</td>
</tr>
<tr>
<td>1236</td>
<td>C2S.BLK.BOTTONS_MOLE</td>
<td>366.807</td>
<td>KMOL/HR</td>
<td>Calculated</td>
</tr>
<tr>
<td>1237</td>
<td>C2S.BLK.BOTTONS_MASS</td>
<td>1099.5</td>
<td>KG/M</td>
<td>Calculated</td>
</tr>
<tr>
<td>1238</td>
<td>C2S.BLK.BOTTONS_STDV</td>
<td>21.0753</td>
<td>CM</td>
<td>Calculated</td>
</tr>
<tr>
<td>1239</td>
<td>C2S.BLK.REFL_RATIO_MOLE</td>
<td>3.99995</td>
<td>UNITLESS</td>
<td>Calculated</td>
</tr>
<tr>
<td>1240</td>
<td>C2S.BLK.REFL_RATIO_MASS</td>
<td>3.99995</td>
<td>UNITLESS</td>
<td>Calculated</td>
</tr>
<tr>
<td>1241</td>
<td>C2S.BLK.REFL_RATIO_STDV</td>
<td>3.99995</td>
<td>UNITLESS</td>
<td>Calculated</td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2S.D.STR.C2H6</td>
<td>0.0001</td>
</tr>
<tr>
<td>C2S.B.STR.C2H4</td>
<td>0.015</td>
</tr>
</tbody>
</table>

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:

---
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.

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

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

<table>
<thead>
<tr>
<th>Index</th>
<th>Variable</th>
<th>Value</th>
<th>Units</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>1233</td>
<td>C2S.BLK.DISTILLATE_MOLE</td>
<td>1400.42</td>
<td>KMOL/HR</td>
<td>Calculated</td>
</tr>
<tr>
<td>1234</td>
<td>C2S.BLK.DISTILLATE_MASS</td>
<td>39237.4</td>
<td>KG/HR</td>
<td>Calculated</td>
</tr>
<tr>
<td>1235</td>
<td>C2S.BLK.DISTILLATE_STDV</td>
<td>118.632</td>
<td>CUM/HR</td>
<td>Calculated</td>
</tr>
<tr>
<td>1236</td>
<td>C2S.BLK.BOTTONS_MOLE</td>
<td>356.617</td>
<td>KMOL/HR</td>
<td>Calculated</td>
</tr>
<tr>
<td>1237</td>
<td>C2S.BLK.BOTTONS_MASS</td>
<td>10712.6</td>
<td>KG/HR</td>
<td>Calculated</td>
</tr>
<tr>
<td>1238</td>
<td>C2S.BLK.BOTTONS_STDV</td>
<td>30.206</td>
<td>CUM/HR</td>
<td>Calculated</td>
</tr>
<tr>
<td>1239</td>
<td>C2S.BLK.REFL_RATIO_MOLE</td>
<td>3.51276</td>
<td>UNITLESS</td>
<td>Calculated</td>
</tr>
<tr>
<td>1240</td>
<td>C2S.BLK.REFL_RATIO_MASS</td>
<td>3.51276</td>
<td>UNITLESS</td>
<td>Calculated</td>
</tr>
<tr>
<td>1241</td>
<td>C2S.BLK.REFL_RATIO_STDV</td>
<td>3.51276</td>
<td>UNITLESS</td>
<td>Calculated</td>
</tr>
</tbody>
</table>

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

![Material Table]

**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:

<table>
<thead>
<tr>
<th>Feed Variable</th>
<th>Tower Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>F.BLK.MOLES</td>
<td>C2S.F.STR.MOLES</td>
<td>Stream molar flow</td>
</tr>
<tr>
<td>F.BLK.TEMP</td>
<td>C2S.F.STR.TEMP</td>
<td>Stream temperature</td>
</tr>
<tr>
<td>F.BLK.PRES</td>
<td>C2S.F.STR.PRES</td>
<td>Stream pressure</td>
</tr>
<tr>
<td>F.BLK.ENTH</td>
<td>C2S.F.STR.ENTH</td>
<td>Stream specific enthalpy</td>
</tr>
<tr>
<td>F.BLK.MVOL</td>
<td>C2S.F.STR.MVOL</td>
<td>Stream molar volume</td>
</tr>
<tr>
<td>F.BLK.C2H4</td>
<td>C2S.F.STR.C2H4</td>
<td>Stream ethylene mole fraction</td>
</tr>
<tr>
<td>F.BLK.C2H6</td>
<td>C2S.F.STR.C2H6</td>
<td>Stream ethane mole fraction</td>
</tr>
</tbody>
</table>

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:

![Flowsheet View (SM view)](image)

![Internal EO View](image)

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:

\[ \text{Objective} = \sum \text{Variable} \times \text{Cost} \]

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.

<table>
<thead>
<tr>
<th>Term</th>
<th>Variable</th>
<th>Cost</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2PROD</td>
<td>C2S.BLK.DISTILLATE_MASS</td>
<td>0.4</td>
<td>$/KG</td>
</tr>
<tr>
<td>C2REC</td>
<td>C2S.BLK.BOTTOMS_MASS</td>
<td>0.1</td>
<td>$/KG</td>
</tr>
<tr>
<td>C2DUTY</td>
<td>C2S.QHOT.STR.HEAT</td>
<td>-450.</td>
<td>$/MMKCAL</td>
</tr>
</tbody>
</table>

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:

![Image of EO Configuration Setup](image)

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:

\[
C2PROD \times 0.4 + C2REC \times 0.1 - C2DUTY \times 450 \approx 10,566 \text{ $/HR.}
\]

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.
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:

<table>
<thead>
<tr>
<th>Variable</th>
<th>Lower</th>
<th>Upper</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2S.D.STR.C2H6</td>
<td>0.00001</td>
<td>0.0002</td>
</tr>
<tr>
<td>C2S.B.STR.C2H4</td>
<td>0.001</td>
<td>0.05</td>
</tr>
</tbody>
</table>
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.

<table>
<thead>
<tr>
<th>Index</th>
<th>Variable</th>
<th>Value</th>
<th>Units</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>C2S,D,STR,C3H6</td>
<td>0.0002</td>
<td>FRACTION</td>
<td>Optimized</td>
</tr>
<tr>
<td>20</td>
<td>C2S,B,STR,C2H4</td>
<td>0.00729951</td>
<td>FRACTION</td>
<td>Optimized</td>
</tr>
<tr>
<td>41</td>
<td>C2S,BLK,EFF_1</td>
<td>0.9</td>
<td>UNITLESS</td>
<td>Constant</td>
</tr>
<tr>
<td>1251</td>
<td>C2S,BLK,PSPEC_1</td>
<td>20</td>
<td>BAR</td>
<td>Constant</td>
</tr>
<tr>
<td>1252</td>
<td>C2S,BLK,PSPEC_2</td>
<td>20.5</td>
<td>BAR</td>
<td>Constant</td>
</tr>
<tr>
<td>1253</td>
<td>C2S,BLK,PSPEC_60</td>
<td>21</td>
<td>BAR</td>
<td>Constant</td>
</tr>
<tr>
<td>1254</td>
<td>C2S,BLK,PSPEC_100</td>
<td>21.5</td>
<td>BAR</td>
<td>Constant</td>
</tr>
<tr>
<td>1259</td>
<td>F.BLK.MASS</td>
<td>50000</td>
<td>KG/MOL</td>
<td>Constant</td>
</tr>
<tr>
<td>1262</td>
<td>F.BLK,C2H4_MOLE_FRAQ</td>
<td>0.0</td>
<td>FRACTION</td>
<td>Constant</td>
</tr>
<tr>
<td>1263</td>
<td>F.BLK,C2H6_MOLE_FRAQ</td>
<td>0.2</td>
<td>FRACTION</td>
<td>Constant</td>
</tr>
<tr>
<td>1266</td>
<td>F.BLK.TEMP</td>
<td>25</td>
<td>°C</td>
<td>Constant</td>
</tr>
<tr>
<td>1267</td>
<td>F.BLK.PRES</td>
<td>25</td>
<td>BAR</td>
<td>Constant</td>
</tr>
<tr>
<td>1272</td>
<td>F.BLK.SUM</td>
<td>1</td>
<td>FRACTION</td>
<td>Constant</td>
</tr>
</tbody>
</table>

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.
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.
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:

![Process Flowsheet Diagram]

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:

<table>
<thead>
<tr>
<th>Field</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vapor fraction</td>
<td>0</td>
</tr>
<tr>
<td>Pressure</td>
<td>1.5 Bar</td>
</tr>
<tr>
<td>Total flow</td>
<td>Mass 150,000 kg/hr</td>
</tr>
<tr>
<td>Composition</td>
<td>Mole-Frac</td>
</tr>
<tr>
<td>Component C3H6</td>
<td>1.0</td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Field</th>
<th>Value 1</th>
<th>Value 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet hot stream</td>
<td>Temperature</td>
<td>-30</td>
</tr>
<tr>
<td>Inlet cold stream</td>
<td>Temperature</td>
<td>-40</td>
</tr>
<tr>
<td>Outlet hot stream</td>
<td>Temperature</td>
<td>-30</td>
</tr>
<tr>
<td>Outlet cold stream</td>
<td>Temperature</td>
<td>-40</td>
</tr>
</tbody>
</table>

   **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 \( \rightarrow \) 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 | Component 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:

<table>
<thead>
<tr>
<th>Variable</th>
<th>User Spec</th>
</tr>
</thead>
<tbody>
<tr>
<td>CVAP.BLK.COUT_VAPOR_FRACTION</td>
<td>Constant</td>
</tr>
<tr>
<td>CIN.BLK.MASS</td>
<td>Calculated</td>
</tr>
</tbody>
</table>
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:

<table>
<thead>
<tr>
<th>Variable or alias</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>CVAP.BLK.COUT_VAPOR_FRACTION</td>
<td>1</td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Name</th>
<th>Destination</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>THIN</td>
<td>CONDUA.BLK.H_IN_TEMP</td>
<td>C2S.BLK.TEMP_2</td>
</tr>
<tr>
<td>THOUT</td>
<td>CONDUA.BLK.H_OUT_TEMP</td>
<td>C2S.BLK.TEMP_1</td>
</tr>
<tr>
<td>TCIN</td>
<td>CONDUA.BLK.C_IN_TEMP</td>
<td>CVAP.BLK.COUT_TEMP</td>
</tr>
<tr>
<td>TCOUT</td>
<td>CONDUA.BLK.C_OUT_TEMP</td>
<td>CVAP.BLK.COUT_TEMP</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Index</th>
<th>Variable</th>
<th>Value</th>
<th>Units</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>C2S.D.STR.C2H5</td>
<td>0.0001</td>
<td>FRACTION</td>
<td>Optimized</td>
</tr>
<tr>
<td>20</td>
<td>C2S.E.STR.C2H5</td>
<td>0.015</td>
<td>FRACTION</td>
<td>Optimized</td>
</tr>
<tr>
<td>41</td>
<td>C2S.BLK.EFF_1</td>
<td>0.9</td>
<td>UNITLESS</td>
<td>Constant</td>
</tr>
<tr>
<td>1251</td>
<td>C2S.BLK.PSPEC_1</td>
<td>20</td>
<td>BAR</td>
<td>Constant</td>
</tr>
<tr>
<td>1252</td>
<td>C2S.BLK.PSPEC_2</td>
<td>20.5</td>
<td>BAR</td>
<td>Constant</td>
</tr>
<tr>
<td>1253</td>
<td>C2S.BLK.PSPEC_80</td>
<td>21</td>
<td>BAR</td>
<td>Constant</td>
</tr>
<tr>
<td>1254</td>
<td>C2S.BLK.PSPEC_100</td>
<td>21.5</td>
<td>BAR</td>
<td>Constant</td>
</tr>
<tr>
<td>1276</td>
<td>CYAP.BLK.PROP</td>
<td>0.1</td>
<td>BAR</td>
<td>Constant</td>
</tr>
<tr>
<td>1276</td>
<td>CYAP.BLK.OUT_VAPOR_FRACTION</td>
<td>1</td>
<td>UNITLESS</td>
<td>Constant</td>
</tr>
<tr>
<td>1307</td>
<td>CONDUA.BLK.U</td>
<td>30000</td>
<td>KCAL/MR-SQM</td>
<td>Constant</td>
</tr>
<tr>
<td>1308</td>
<td>CONDUA.BLK.FT</td>
<td>1</td>
<td>UNITLESS</td>
<td>Constant</td>
</tr>
<tr>
<td>1316</td>
<td>CHN.BLK.C2H6_MOLE_FRACTION</td>
<td>1</td>
<td>FRACTION</td>
<td>Constant</td>
</tr>
<tr>
<td>1319</td>
<td>CHN.BLK.PRES</td>
<td>1.5</td>
<td>BAR</td>
<td>Constant</td>
</tr>
<tr>
<td>1235</td>
<td>CHN.BLK.SUM</td>
<td>1</td>
<td>FRACTION</td>
<td>Constant</td>
</tr>
<tr>
<td>1226</td>
<td>CHN.BLK.VAPOR_FRACTION</td>
<td>-9.4e-05</td>
<td>UNITLESS</td>
<td>Constant</td>
</tr>
<tr>
<td>1347</td>
<td>F.BLK.MASS</td>
<td>50000</td>
<td>KG/MR</td>
<td>Constant</td>
</tr>
<tr>
<td>1350</td>
<td>F.BLK.C2H5_MOLE_FRACTION</td>
<td>0.8</td>
<td>FRACTION</td>
<td>Constant</td>
</tr>
<tr>
<td>1351</td>
<td>F.BLK.C2H6_MOLE_FRACTION</td>
<td>0.2</td>
<td>FRACTION</td>
<td>Constant</td>
</tr>
<tr>
<td>1354</td>
<td>F.BLK.TEMP</td>
<td>25</td>
<td>C</td>
<td>Constant</td>
</tr>
<tr>
<td>1355</td>
<td>F.BLK.PRES</td>
<td>25</td>
<td>BAR</td>
<td>Constant</td>
</tr>
<tr>
<td>1360</td>
<td>F.BLK.SUM</td>
<td>1</td>
<td>FRACTION</td>
<td>Constant</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Index</th>
<th>Variable</th>
<th>Value</th>
<th>Units</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>1300</td>
<td>CONDUA.BLK.H1_IN_TEMP</td>
<td>-20.3145</td>
<td>C</td>
<td>Calculated</td>
</tr>
<tr>
<td>1301</td>
<td>CONDUA.BLK.H1_OUT_TEMP</td>
<td>-29.2114</td>
<td>C</td>
<td>Calculated</td>
</tr>
<tr>
<td>1302</td>
<td>CONDUA.BLK.C1_IN_TEMP</td>
<td>-40.1263</td>
<td>C</td>
<td>Calculated</td>
</tr>
<tr>
<td>1303</td>
<td>CONDUA.BLK.C1_OUT_TEMP</td>
<td>-40.1263</td>
<td>C</td>
<td>Calculated</td>
</tr>
<tr>
<td>1304</td>
<td>CONDUA.BLK.HOT_IN_APPR_TEMP</td>
<td>11.8116</td>
<td>DELTA-C</td>
<td>Calculated</td>
</tr>
<tr>
<td>1305</td>
<td>CONDUA.BLK.HOT_OUT_APPR_TEMP</td>
<td>10.9149</td>
<td>DELTA-C</td>
<td>Calculated</td>
</tr>
<tr>
<td>1306</td>
<td>CONDUA.BLK.LMTD</td>
<td>11.3576</td>
<td>DELTA-C</td>
<td>Calculated</td>
</tr>
<tr>
<td>1308</td>
<td>CONDUA.BLK.FTU</td>
<td>30000</td>
<td>KCAL/MR-SQM</td>
<td>Calculated</td>
</tr>
<tr>
<td>1310</td>
<td>CONDUA.BLK.AREA</td>
<td>40.5678</td>
<td>SQM</td>
<td>Calculated</td>
</tr>
<tr>
<td>1311</td>
<td>CONDUA.BLK.GHOT_HEAT</td>
<td>13.8226</td>
<td>NMKCAL/R</td>
<td>Calculated</td>
</tr>
<tr>
<td>1312</td>
<td>CONDUA.BLK.MASS</td>
<td>133045</td>
<td>KG/MR</td>
<td>Calculated</td>
</tr>
</tbody>
</table>

4. Go to the Blocks | CONDUA | Results | Convective sheet to examine the results listed in another format.
Go to the **Results Summary** | **Streams** | **Material** sheet to examine flow rates and temperatures.

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:

<table>
<thead>
<tr>
<th>Term</th>
<th>Variable</th>
<th>Cost</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>C3R</td>
<td>CIN.BLK.MASS</td>
<td>-0.05</td>
<td>$/KG</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Index</th>
<th>Variable</th>
<th>Value</th>
<th>Units</th>
<th>Specification</th>
<th>Lower Bound</th>
<th>Upper Bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>C5S EL STR.COH2</td>
<td>0.0002</td>
<td>FRACTION</td>
<td>Optimized</td>
<td>0.0005</td>
<td>0.0005</td>
</tr>
<tr>
<td>15</td>
<td>C6S EL STR.COH4</td>
<td>0.0073</td>
<td>FRACTION</td>
<td>Optimized</td>
<td>0.001</td>
<td>0.05</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Summary</th>
<th>Term Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Objective function results</td>
<td>Maximise</td>
</tr>
<tr>
<td>Direction:</td>
<td></td>
</tr>
<tr>
<td>Current value:</td>
<td>10.3032746</td>
</tr>
<tr>
<td>Initial value:</td>
<td>10093.9893</td>
</tr>
<tr>
<td>Change:</td>
<td>209285291</td>
</tr>
<tr>
<td>Scale:</td>
<td>1</td>
</tr>
<tr>
<td>UOM:</td>
<td>$/HR</td>
</tr>
</tbody>
</table>

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:

\[ \text{offset} = \text{plant} - \text{model} \]

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

\[ r = \text{plant} - \text{model} - \text{offset} \]

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:

\[ \text{blockid.BLK.tag\_description\_variable} \]

Where:
- \textit{blockid} is the name of the measurement block.
- \textit{tag} is the tag specified for each measurement.
- \textit{description} is the description provided for each measurement.
- \textit{variable} is PLANT, MODEL, or Offset.

If the description is not provided, the variables have shorter names in the form \textit{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**

<table>
<thead>
<tr>
<th>Calculation Option</th>
<th>Source</th>
<th>Model</th>
<th>Plant</th>
<th>Offset</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calc-Model</td>
<td>Constant</td>
<td>Calculated</td>
<td>Constant</td>
<td>Constant</td>
</tr>
<tr>
<td>Calc-Offset*</td>
<td>Calculated</td>
<td>Constant</td>
<td>Calculated</td>
<td>Calculated</td>
</tr>
<tr>
<td>Calc-Plant</td>
<td>Calculated</td>
<td>Constant</td>
<td>Calculated</td>
<td>Constant</td>
</tr>
<tr>
<td>Param-Offset</td>
<td>Calculated</td>
<td>Constant</td>
<td>Measured</td>
<td>Parameterized</td>
</tr>
</tbody>
</table>

*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

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Calculated</td>
<td>Measured</td>
<td>Parameterized</td>
</tr>
<tr>
<td>Constant</td>
<td>Constant</td>
<td>Constant</td>
</tr>
<tr>
<td>Measured</td>
<td>Measured</td>
<td>Constant</td>
</tr>
<tr>
<td>Parameterized</td>
<td>Constant</td>
<td>Parameterized</td>
</tr>
<tr>
<td>Optimized</td>
<td>Optimized</td>
<td>Constant</td>
</tr>
<tr>
<td>Reconciled</td>
<td>Constant</td>
<td>Reconciled</td>
</tr>
<tr>
<td>Independent</td>
<td>Optimized</td>
<td>Reconciled</td>
</tr>
</tbody>
</table>

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.
6. The Create New ID dialog box appears.
7. Type C2MEAS and click OK.
8. The Flowsheeting Options | Measurement | C2MEAS | Input | Measurements sheet appears.
9. 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:

<table>
<thead>
<tr>
<th>Index</th>
<th>Tag</th>
<th>Open Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>F</td>
<td>F.BLK.MASS</td>
</tr>
<tr>
<td>2</td>
<td>XF</td>
<td>F.BLK.C2H6_MOLE_FRAC</td>
</tr>
<tr>
<td>3</td>
<td>D</td>
<td>C2S.BLK.DISTILLATE_MASS</td>
</tr>
<tr>
<td>4</td>
<td>B</td>
<td>C2S.BLK.BOTTOMS_MASS</td>
</tr>
<tr>
<td>5</td>
<td>RR</td>
<td>C2S.BLK.REFL_RATIO_MASS</td>
</tr>
<tr>
<td>6</td>
<td>XD</td>
<td>C2S.D.STR.C2H6</td>
</tr>
<tr>
<td>7</td>
<td>XB</td>
<td>C2S.B.STR.C2H4</td>
</tr>
<tr>
<td>8</td>
<td>C3R</td>
<td>CIN.BLK.MASS</td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Measurement</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>F</td>
<td>Constant</td>
</tr>
<tr>
<td>XF</td>
<td>Constant</td>
</tr>
<tr>
<td>XD</td>
<td>Optimized</td>
</tr>
<tr>
<td>XB</td>
<td>Optimized</td>
</tr>
<tr>
<td>D</td>
<td>Calculated</td>
</tr>
<tr>
<td>B</td>
<td>Calculated</td>
</tr>
<tr>
<td>RR</td>
<td>Calculated</td>
</tr>
<tr>
<td>C3R</td>
<td>Calculated</td>
</tr>
</tbody>
</table>

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:
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**:

<table>
<thead>
<tr>
<th>Variable</th>
<th>User Spec</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2MEAS.BLK.XD_MODEL</td>
<td>Calculated</td>
</tr>
<tr>
<td>C2MEAS.BLK.XD_PLANT</td>
<td>Optimized</td>
</tr>
<tr>
<td>C2MEAS.BLK.XD_OFFSET</td>
<td>Constant</td>
</tr>
<tr>
<td>C2MEAS.BLK.XB_MODEL</td>
<td>Calculated</td>
</tr>
<tr>
<td>C2MEAS.BLK.XB_PLANT</td>
<td>Optimized</td>
</tr>
<tr>
<td>C2MEAS.BLK.XB_OFFSET</td>
<td>Constant</td>
</tr>
<tr>
<td>C2MEAS.BLK.F_MODEL</td>
<td>Calculated</td>
</tr>
<tr>
<td>C2MEAS.BLK.F_PLANT</td>
<td>Constant</td>
</tr>
<tr>
<td>C2MEAS.BLK.F_OFFSET</td>
<td>Constant</td>
</tr>
<tr>
<td>C2MEAS.BLK.XF_MODEL</td>
<td>Calculated</td>
</tr>
<tr>
<td>C2MEAS.BLK.XF_PLANT</td>
<td>Constant</td>
</tr>
<tr>
<td>C2MEAS.BLK.XF_OFFSET</td>
<td>Constant</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Change this</th>
<th>To this</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2S.D.STR.C2H6</td>
<td>C2MEAS.BLK.XD_PLANT</td>
</tr>
<tr>
<td>C2S.B.STR.C2H4</td>
<td>C2MEAS.BLK.XB_PLANT</td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Variable or alias</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2MEAS.BLK.F_PLANT</td>
<td>50000</td>
</tr>
<tr>
<td>C2MEAS.BLK.XF_PLANT</td>
<td>0.2</td>
</tr>
<tr>
<td>C2MEAS.BLK.D_PLANT</td>
<td>41000</td>
</tr>
<tr>
<td>C2MEAS.BLK.B_PLANT</td>
<td>12000</td>
</tr>
<tr>
<td>C2MEAS.BLK.RR_PLANT</td>
<td>4.3</td>
</tr>
<tr>
<td>C2MEAS.BLK.C3R_PLANT</td>
<td>140000</td>
</tr>
</tbody>
</table>
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.

<table>
<thead>
<tr>
<th>Index</th>
<th>Variable</th>
<th>Value</th>
<th>Units</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>1386</td>
<td>C2MEAS.BLK.F_PLANT</td>
<td>50000</td>
<td>KGRAH</td>
<td>Constant</td>
</tr>
<tr>
<td>1387</td>
<td>C2MEAS.BLK.F_MODEL</td>
<td>50000</td>
<td>KGRAH</td>
<td>Calculated</td>
</tr>
<tr>
<td>1390</td>
<td>C2MEAS.BLK.F_OFFSET</td>
<td>0</td>
<td>KGRAH</td>
<td>Constant</td>
</tr>
<tr>
<td>1391</td>
<td>C2MEAS.BLK.XF_PLANT</td>
<td>3.2</td>
<td>FRACTION</td>
<td>Constant</td>
</tr>
<tr>
<td>1392</td>
<td>C2MEAS.BLK.XF_MODEL</td>
<td>0</td>
<td>FRACTION</td>
<td>Calculated</td>
</tr>
<tr>
<td>1393</td>
<td>C2MEAS.BLK.XF_OFFSET</td>
<td>0</td>
<td>FRACTION</td>
<td>Constant</td>
</tr>
<tr>
<td>1394</td>
<td>C2MEAS.BLK.D.PLANT</td>
<td>41000</td>
<td>KGRAH</td>
<td>Measured</td>
</tr>
<tr>
<td>1395</td>
<td>C2MEAS.BLK.D.MODEL</td>
<td>36000.5</td>
<td>KGRAH</td>
<td>Calculated</td>
</tr>
<tr>
<td>1396</td>
<td>C2MEAS.BLK.D_OFFSET</td>
<td>0</td>
<td>KGRAH</td>
<td>Parameterized</td>
</tr>
<tr>
<td>1397</td>
<td>C2MEAS.BLK.B.PLANT</td>
<td>12000</td>
<td>KGRAH</td>
<td>Measured</td>
</tr>
<tr>
<td>1398</td>
<td>C2MEAS.BLK.B.MODEL</td>
<td>11000</td>
<td>KGRAH</td>
<td>Calculated</td>
</tr>
<tr>
<td>1399</td>
<td>C2MEAS.BLK.B_OFFSET</td>
<td>0</td>
<td>KGRAH</td>
<td>Parameterized</td>
</tr>
<tr>
<td>1400</td>
<td>C2MEAS.BLK.RR.PLANT</td>
<td>4.3</td>
<td>UNITLESS</td>
<td>Measured</td>
</tr>
<tr>
<td>1401</td>
<td>C2MEAS.BLK.RR_MODEL</td>
<td>3.39995</td>
<td>UNITLESS</td>
<td>Calculated</td>
</tr>
<tr>
<td>1402</td>
<td>C2MEAS.BLK.RR_OFFSET</td>
<td>0</td>
<td>UNITLESS</td>
<td>Parameterized</td>
</tr>
<tr>
<td>1403</td>
<td>C2MEAS.BLK.XD.PLANT</td>
<td>0.0001</td>
<td>FRACTION</td>
<td>Optimized</td>
</tr>
<tr>
<td>1404</td>
<td>C2MEAS.BLK.XD_MODEL</td>
<td>1.55632E-005</td>
<td>FRACTION</td>
<td>Calculated</td>
</tr>
<tr>
<td>1405</td>
<td>C2MEAS.BLK.XD_OFFSET</td>
<td>0</td>
<td>FRACTION</td>
<td>Constant</td>
</tr>
<tr>
<td>1406</td>
<td>C2MEAS.BLK.XB.PLANT</td>
<td>0.015</td>
<td>FRACTION</td>
<td>Optimized</td>
</tr>
<tr>
<td>1407</td>
<td>C2MEAS.BLK.XB.MODEL</td>
<td>0.0421678</td>
<td>FRACTION</td>
<td>Calculated</td>
</tr>
<tr>
<td>1408</td>
<td>C2MEAS.BLK.XB_OFFSET</td>
<td>0</td>
<td>FRACTION</td>
<td>Constant</td>
</tr>
<tr>
<td>1409</td>
<td>C2MEAS.BLK.C3R.PLANT</td>
<td>14000</td>
<td>KGRAH</td>
<td>Measured</td>
</tr>
<tr>
<td>1410</td>
<td>C2MEAS.BLK.C3R_MODEL</td>
<td>15000</td>
<td>KGRAH</td>
<td>Calculated</td>
</tr>
<tr>
<td>1411</td>
<td>C2MEAS.BLK.C3R_OFFSET</td>
<td>0</td>
<td>KGRAH</td>
<td>Parameterized</td>
</tr>
</tbody>
</table>

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.
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:

<table>
<thead>
<tr>
<th>Measurement</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>F</td>
<td>Parameterized</td>
</tr>
<tr>
<td>XF</td>
<td>Parameterized</td>
</tr>
<tr>
<td>XD</td>
<td>Optimized</td>
</tr>
<tr>
<td>XB</td>
<td>Optimized</td>
</tr>
<tr>
<td>D</td>
<td>Measured</td>
</tr>
<tr>
<td>B</td>
<td>Measured</td>
</tr>
<tr>
<td>RR</td>
<td>Measured</td>
</tr>
<tr>
<td>C3R</td>
<td>Calculated</td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Variable</th>
<th>User Spec</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2MEAS.BLK.F_PLANT</td>
<td>Constant</td>
</tr>
<tr>
<td>C2MEAS.BLK.F_OFFSET</td>
<td>Parameterized</td>
</tr>
<tr>
<td>C2MEAS.BLK.XF_PLANT</td>
<td>Constant</td>
</tr>
<tr>
<td>C2MEAS.BLK.XF_OFFSET</td>
<td>Parameterized</td>
</tr>
<tr>
<td>C2MEAS.BLK.D_PLANT</td>
<td>Measured</td>
</tr>
<tr>
<td>C2MEAS.BLK.D_OFFSET</td>
<td>Constant</td>
</tr>
<tr>
<td>C2MEAS.BLK.B_PLANT</td>
<td>Measured</td>
</tr>
<tr>
<td>C2MEAS.BLK.B_OFFSET</td>
<td>Constant</td>
</tr>
<tr>
<td>C2MEAS.BLK.RR_PLANT</td>
<td>Measured</td>
</tr>
<tr>
<td>C2MEAS.BLK.RR_OFFSET</td>
<td>Constant</td>
</tr>
<tr>
<td>C2S.BLK.EFF_1</td>
<td>Parameterized</td>
</tr>
</tbody>
</table>

6. Click Close.
   - The EO Configuration | Spec Groups | Specifications sheet reappears:

![Specifications Table]

- Spec group: C2COMPS, Status: Active, Enabled: ✔, Variables: Var=C2S.D.STR.C2H6, User Spec
- Spec group: C3RVFRAC, Status: Active, Enabled: ✔, Variables: Var=CVAP.BLK.COUT_VAPOR
- Spec group: TYPSPEC, Status: Active, Enabled: ✔, Variables: Var=C2MEAS.BLK.XD_MODEL
- Spec group: PARSPEC, Status: , Enabled: ✔, Variables: Var=C2MEAS.BLK.F_PLANT, User Spec

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.
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.

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

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.
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


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


   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 \( \text{Control Panel} \) to open the Control Panel.

2. In the Control Panel, select \textbf{Sequential Modular} for the \textbf{Solution Strategy}.

3. Press \textbf{Shift-F5} and click \textbf{OK} twice to reinitialize the simulation.

4. On the Control Panel toolbar, click \( \text{Run} \) to run the simulation.

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

   When the calculations are complete, the message \textit{Results Available} appears in the lower right corner of the Aspen Plus window.

5. In the \textbf{Solution Strategy} field, change \textbf{Sequential Modular} to \textbf{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:

<table>
<thead>
<tr>
<th>Measurement</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>F</td>
<td>Reconciled</td>
</tr>
<tr>
<td>XF</td>
<td>Reconciled</td>
</tr>
<tr>
<td>XD</td>
<td>Independent</td>
</tr>
<tr>
<td>XB</td>
<td>Independent</td>
</tr>
<tr>
<td>D</td>
<td>Calculated</td>
</tr>
<tr>
<td>B</td>
<td>Calculated</td>
</tr>
<tr>
<td>RR</td>
<td>Calculated</td>
</tr>
<tr>
<td>C3R</td>
<td>Calculated</td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Variable</th>
<th>User Spec</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2MEAS.BLK.F_PLANT</td>
<td>Constant</td>
</tr>
<tr>
<td>C2MEAS.BLK.F_OFFSET</td>
<td>Reconciled</td>
</tr>
<tr>
<td>C2MEAS.BLK.XF_PLANT</td>
<td>Constant</td>
</tr>
<tr>
<td>C2MEAS.BLK.XF_OFFSET</td>
<td>Reconciled</td>
</tr>
<tr>
<td>C2MEAS.BLK.XD_PLANT</td>
<td>Optimized</td>
</tr>
<tr>
<td>C2MEAS.BLK.XD_OFFSET</td>
<td>Reconciled</td>
</tr>
<tr>
<td>C2MEAS.BLK.XB_PLANT</td>
<td>Optimized</td>
</tr>
<tr>
<td>C2MEAS.BLK.XB_OFFSET</td>
<td>Reconciled</td>
</tr>
<tr>
<td>C2S.BLK.EFF_1</td>
<td>Reconciled</td>
</tr>
</tbody>
</table>

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:

\[ \text{Objective} = \sum (\frac{\text{Offset} - \text{Mean}}{\sigma})^2 \]

Where:
- \( \text{Offset} \) is the measurement offset.
- \( \text{Mean} \) is a mean or average value for the offset, normally zero.
- \( \sigma \) 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 \textit{EO Configuration | Objective} folder.
2. Click \textit{Add} to add a new objective function.
   The \textit{Create new ID} dialog box appears.
3. Enter \textit{RECERR} for the ID, and choose the \textit{SUMOFSQUARES} type.
4. Click \textit{OK}.
   The \textit{EO Configuration | Objective | RECERR | Input | Setup} form appears.
5. Enter the following information. Also enter zero for the \textit{Mean} of each term.

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

\( \text{Note: You must enter the Physical Type for each variable before specifying the Units.} \)

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

The \textit{EO Configuration | Objective | RECERR | Input | Setup} sheet is complete:
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.

<table>
<thead>
<tr>
<th>Index</th>
<th>Variable</th>
<th>Value</th>
<th>Units</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>1336</td>
<td>C2MEAS.BLK.F_PLANNT</td>
<td>50030</td>
<td>KGR-R</td>
<td>Constant</td>
</tr>
<tr>
<td>1337</td>
<td>C2MEAS.BLK.F.MODEL</td>
<td>51053.7</td>
<td>KGR-R</td>
<td>Calculated</td>
</tr>
<tr>
<td>1338</td>
<td>C2MEAS.BLK.F_OFFSET</td>
<td>1053.73</td>
<td>KGR-R</td>
<td>Reconciled</td>
</tr>
<tr>
<td>1339</td>
<td>C2MEAS.BLK.XF_PLANNT</td>
<td>0.2</td>
<td>FRACT</td>
<td>Constant</td>
</tr>
<tr>
<td>1340</td>
<td>C2MEAS.BLK.XF.MODEL</td>
<td>0.210069</td>
<td>FRACT</td>
<td>Calculated</td>
</tr>
<tr>
<td>1341</td>
<td>C2MEAS.BLK.XF_OFFSET</td>
<td>-0.018004</td>
<td>FRACT</td>
<td>Reconciled</td>
</tr>
<tr>
<td>1342</td>
<td>C2MEAS.BLK.D_PLANNT</td>
<td>41000</td>
<td>KGR-R</td>
<td>Measured</td>
</tr>
<tr>
<td>1343</td>
<td>C2MEAS.BLK.D_MODEL</td>
<td>39350.5</td>
<td>KGR-R</td>
<td>Calculated</td>
</tr>
<tr>
<td>1344</td>
<td>C2MEAS.BLK.D_OFFSET</td>
<td>1649.5</td>
<td>KGR-R</td>
<td>Parameterized</td>
</tr>
<tr>
<td>1345</td>
<td>C2MEAS.BLK.B_PLANNT</td>
<td>12000</td>
<td>KGR-R</td>
<td>Measured</td>
</tr>
<tr>
<td>1346</td>
<td>C2MEAS.BLK.B_MODEL</td>
<td>11733.2</td>
<td>KGR-R</td>
<td>Calculated</td>
</tr>
<tr>
<td>1347</td>
<td>C2MEAS.BLK.B_OFFSET</td>
<td>296.772</td>
<td>KGR-R</td>
<td>Parameterized</td>
</tr>
<tr>
<td>1400</td>
<td>C2MEAS.BLK.RR_PLANNT</td>
<td>4.3</td>
<td>UNITLES</td>
<td>Measured</td>
</tr>
<tr>
<td>1401</td>
<td>C2MEAS.BLK.RR_MODEL</td>
<td>4.2524</td>
<td>UNITLES</td>
<td>Calculated</td>
</tr>
<tr>
<td>1402</td>
<td>C2MEAS.BLK.RR_OFFSET</td>
<td>0.047837</td>
<td>UNITLES</td>
<td>Parameterized</td>
</tr>
<tr>
<td>1403</td>
<td>C2MEAS.BLK.XD_PLANNT</td>
<td>0.0001</td>
<td>FRACT</td>
<td>Optimized</td>
</tr>
<tr>
<td>1404</td>
<td>C2MEAS.BLK.XD_MODEL</td>
<td>9.7703e-006</td>
<td>FRACT</td>
<td>Calculated</td>
</tr>
<tr>
<td>1405</td>
<td>C2MEAS.BLK.XD_OFFSET</td>
<td>2.2963e-006</td>
<td>UNITLESS</td>
<td>Calculated</td>
</tr>
<tr>
<td>1406</td>
<td>C2MEAS.BLK.XG_PLANNT</td>
<td>0.015</td>
<td>FRACT</td>
<td>Optimized</td>
</tr>
<tr>
<td>1407</td>
<td>C2MEAS.BLK.XG_MODEL</td>
<td>0.0151639</td>
<td>FRACT</td>
<td>Calculated</td>
</tr>
<tr>
<td>1408</td>
<td>C2MEAS.BLK.XG_OFFSET</td>
<td>-0.000199836</td>
<td>FRACT</td>
<td>Reconciled</td>
</tr>
<tr>
<td>1409</td>
<td>C2MEAS.BLK.CRR_PLANNT</td>
<td>140000</td>
<td>KGR-R</td>
<td>Measured</td>
</tr>
<tr>
<td>1410</td>
<td>C2MEAS.BLK.CRR_MODEL</td>
<td>15652.6</td>
<td>KGR-R</td>
<td>Calculated</td>
</tr>
<tr>
<td>1411</td>
<td>C2MEAS.BLK.CRR_OFFSET</td>
<td>-16025.7</td>
<td>KGR-R</td>
<td>Parameterized</td>
</tr>
</tbody>
</table>

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**

<table>
<thead>
<tr>
<th>Index</th>
<th>Variable</th>
<th>Value</th>
<th>Units</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>41</td>
<td>C2S.BLK.EFF_1</td>
<td>0.763257</td>
<td>UNITLES</td>
<td>Reconciled</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th></th>
<th>C2MEAS.BLK.XD_PLANT</th>
<th>0.0002</th>
<th>FRACTION</th>
<th>Optimized</th>
</tr>
</thead>
<tbody>
<tr>
<td>1403</td>
<td>C2MEAS.BLK.XD_MODEL</td>
<td>0.0001677</td>
<td>FRACTION</td>
<td>Calculated</td>
</tr>
<tr>
<td>1404</td>
<td>C2MEAS.BLK.XD_OFFSET</td>
<td>2.28863e-006</td>
<td>FRACTION</td>
<td>Reconciled</td>
</tr>
<tr>
<td>1405</td>
<td>C2MEAS.BLK.XB_PLANT</td>
<td>0.0230519</td>
<td>FRACTION</td>
<td>Optimized</td>
</tr>
<tr>
<td>1406</td>
<td>C2MEAS.BLK.XB_MODEL</td>
<td>0.0234617</td>
<td>FRACTION</td>
<td>Calculated</td>
</tr>
<tr>
<td>1407</td>
<td>C2MEAS.BLK.XB_OFFSET</td>
<td>-0.0001998</td>
<td>FRACTION</td>
<td>Reconciled</td>
</tr>
</tbody>
</table>

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.
After you start the Aspen Plus User Interface, you are prompted for the name of computer running the Aspen Plus simulation engine, if either 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.
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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Corporate
Aspen Technology, Inc.
Ten Canal Park
Cambridge, MA 02141-2201
USA
Phone: (1) (617) 949-1000
Toll Free: (1) (888) 996-7001
Fax: (1) (617) 949-1030
URL: http://www.aspentech.com/

Related Documentation

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<td>Tutorials covering basic use of Aspen Plus. A prerequisite for the other Getting Started guides</td>
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<td>Aspen Plus Getting Started Modeling Petroleum Processes</td>
<td>Tutorials covering the Aspen Plus features designed to handle petroleum</td>
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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.
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• Technical advisories.
• Product updates.
• Service Pack announcements.
• Product release announcements.

Phone and E-mail

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For the most up-to-date phone listings, please see the Online Technical Support Center at:

http://support.aspentech.com

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