Aspen Plus

Getting Started Building and Running a Process Model

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Who Should Read this Guide

This guide is suitable for beginners to the Aspen Plus simulation environment. Users should understand the material in this guide before proceeding to the other Aspen Plus Getting Started Guides.

Introducing Aspen Plus

Aspen Plus makes it easy to build and run a process simulation model by providing you with a comprehensive system of online prompts, hypertext help, and expert system guidance at every step. In many cases, you will be able to develop an Aspen Plus process simulation model without referring to printed manuals.

The seven hands-on sessions show you, step-by-step, how to use the full power and scope of Aspen Plus. Each session requires 30 – 50 minutes.

This guide assumes only that you have an installed copy of Aspen Plus. If you have not installed Aspen Plus, please see the *Aspen Engineering Suite Installation Manual*.

Why Use Process Simulation?

Process simulation allows you to predict the behavior of a process by using basic engineering relationships, such as mass and energy balances, and phase and chemical equilibrium. Given reliable thermodynamic data, realistic operating conditions, and rigorous equipment models, you can simulate actual plant behavior. Process simulation enables you to run many cases, conduct "what if" analyses, and perform sensitivity studies and optimization runs. With simulation, you can design better plants and increase profitability in existing plants.

Process simulation is useful throughout the entire lifecycle of a process, from research and development through process design to production.

What is an Aspen Plus Process Simulation Model?

A process consists of chemical components being mixed, separated, heated, cooled, and converted by unit operations. These components are transferred from unit to unit through process streams.

You can translate a process into an Aspen Plus process simulation model by performing the following steps:

1. Specify the chemical components in the process. You can take these components from the Aspen Plus databanks, or you can define them.
2. Specify thermodynamic models to represent the physical properties of the components and mixtures in the process. These models are built into Aspen Plus.
3. Define the process flowsheet:
   - Define the unit operations in the process.
   - Define the process streams that flow to and from the unit operations.
   - Select models from the Aspen Plus Model Library to describe each unit operation and place them on the process flowsheet.
   - Place labeled streams on the process flowsheet and connect them to the unit operation models.
4. Specify the component flow rates and the thermodynamic conditions (for example, temperature and pressure) of feed streams.
5. Specify the operating conditions for the unit operation models.

With Aspen Plus you can interactively change specifications such as, flowsheet configuration, operating conditions and feed compositions, to run new cases and analyze process alternatives.

In addition to process simulation, Aspen Plus allows you to perform a wide range of other tasks such as estimating and regressing physical properties, generating custom graphical and tabular output results, fitting plant data to simulation models, optimizing your process, and interfacing results to spreadsheets.

Sessions in this Book

The hands-on sessions in this book are described in the following table:

Follow the steps in this chapter	To Learn how to
1 Aspen Plus Basics	Start Aspen Plus, use the Aspen Plus user interface, and exit Aspen Plus.
2 Building and Running a Process Simulation Model	Build and run a typical Aspen Plus process simulation model.
3 Performing a Sensitivity Analysis	Use Aspen Plus to study the sensitivity of process performance to changes in process feeds and operating variables.
4 Meeting Process Design Specifications	Use Aspen Plus to make your process model meet a design specification by manipulating a process feed or operating variable.
5 Annotating Process Flowsheets	Add stream tables, graphics, and text to your process flowsheet.
6 Estimating Physical Properties for a Non-Databank Component	Use Aspen Plus to enter and estimate missing physical properties required for simulation.
7 Analyzing Properties	Use Aspen Plus to generate tables and plots of physical properties, computed over a range of values.

Using Backup Files

We recommend that you perform all sessions sequentially using the results of the previous chapter in the current chapter. However, you can skip chapters and work on the session of your choice using backup files containing simulation data.

Aspen Plus provides backup files (filename.bkp) containing all problem specifications and results for each tutorial session. In some cases, if you skip a session, you need to load a backup file to supply missing data. Each chapter contains instructions for how to do this.

Related Documentation

In addition to this document, a number of other documents are provided to help you learn and use Aspen Plus.

Title	Content
Aspen Plus Getting Started Modeling Processes with Solids	Tutorials covering the Aspen Plus features designed to handle solids
Aspen Plus Getting Started Modeling Processes with Electrolytes	Tutorials covering the Aspen Plus features designed to handle electrolytes
Aspen Plus Getting Started Customizing Unit Operation Models	Tutorials covering the development of custom unit operation models in Aspen Plus
Aspen Plus Getting Started Using Equation Oriented Modeling	Tutorials covering the use of equation-oriented models in Aspen Plus
Aspen Engineering Suite Installation Manual	Instructions for installing Aspen Plus and other Aspen Engineering Suite products
Aspen Plus Help	Procedures for using Aspen Plus

Technical Support

AspenTech customers with a valid license and software maintenance agreement can register to access the online AspenTech Support Center at:

http://support.aspentech.com

This Web support site allows you to:

- Access current product documentation
- Search for tech 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
- Send suggestions
- Report product defects

- Review lists of known deficiencies and defects

Registered users can also subscribe to our Technical Support e-Bulletins. These e-Bulletins are used to alert users to important technical support information such as:

- Technical advisories
- Product updates and releases

Customer support is also available by phone, fax, and email. The most up-to-date contact information is available at the AspenTech Support Center at **http://support.aspentech.com**.

1 Aspen Plus Basics

This chapter leads you through an Aspen Plus simulation to explain how to open a file, enter data, run a simulation, and examine results.

Allow about 30 minutes for this session.

Starting Aspen Plus

1 From your desktop, select **Start** and then select **Programs**.

2 Select **AspenTech**, then **Process Modeling <version>**, then **Aspen Plus**, and then **Aspen Plus <version>**.

The **Aspen Plus** main window appears, showing the **Start Using Aspen Plus** window.

Note: To create a Windows desktop icon for Aspen Plus, right-click **Aspen Plus <version>** via the **Start** menu, click **Copy**, then right-click on your desktop and select **Paste Shortcut**. Double-click the icon to start Aspen Plus.

The Start Using Aspen Plus Window

The **Start Using Aspen Plus** window provides these ways of starting a run:

- New and Open File -- quick access to start a new case or open an existing case.
- Recent Models — links to the recently opened cases.

Opening a File

Open a file for an Aspen Plus simulation by:

- Double-clicking the file in Windows.
- Clicking the file name under **Recent Models** on the **Start Using Aspen Plus** window.
- Clicking **Open File** on the **Start Using Aspen Plus** window.

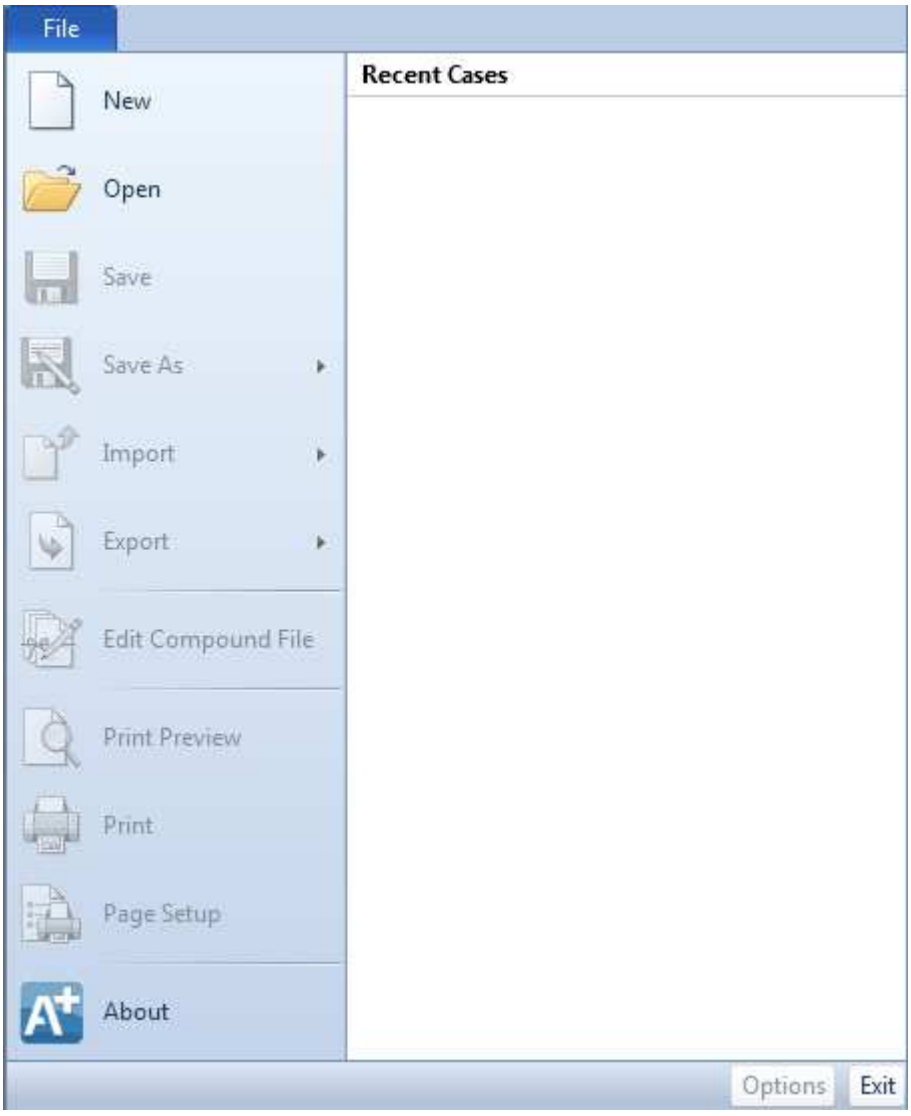
- Selecting **Open** from the **File** menu in Aspen Plus.

In this section, use **Open** on the **File** menu to open a partially completed Aspen Plus simulation stored in a backup file.

Note: This chapter does not describe all the steps necessary to create the partially-completed example file. The following chapters will explain all the steps necessary to set up Aspen Plus from a blank simulation.

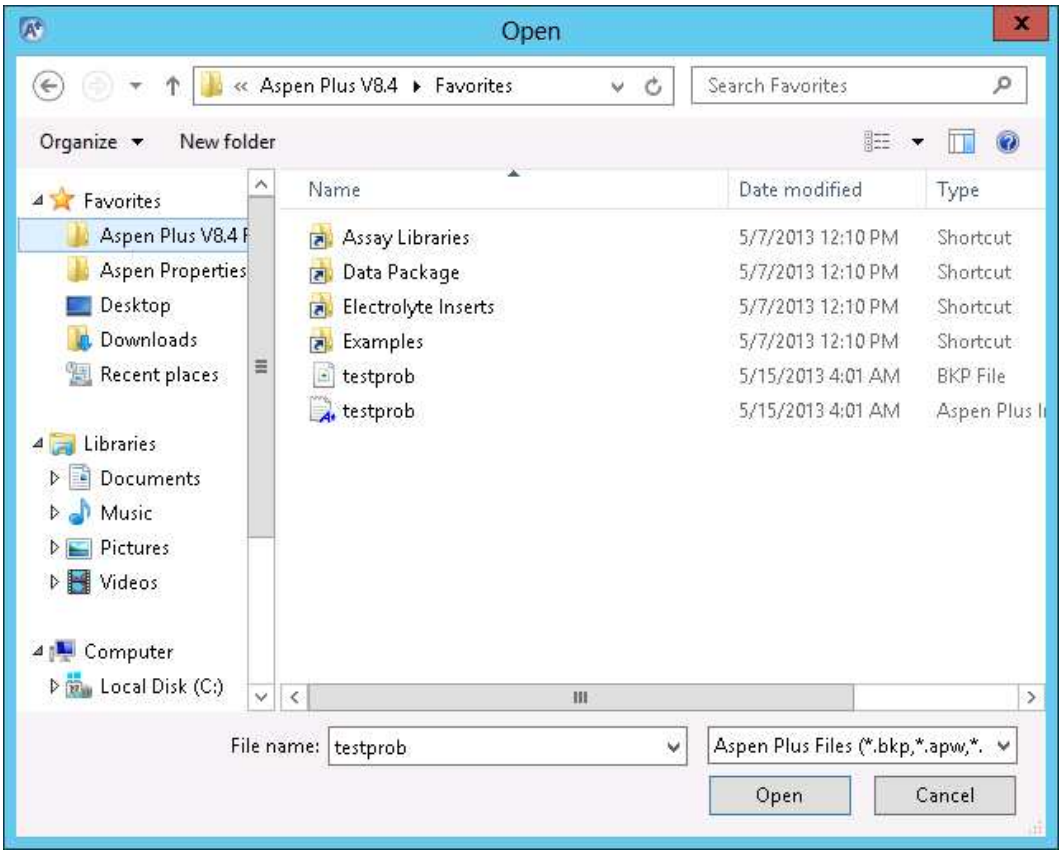
To Display the File Menu

1 Click **File** from the ribbon. The **File** menu appears:



2 From the **File** menu, click **Open**.
The **Open** dialog box appears, displaying your default working directory.

3 Under **Favorites** at the left, click **Aspen Plus** <*version*> **Favorites**.
The Aspen Plus favorites folder appears:



By default, the Aspen Plus favorites folder contains shortcuts to four folders that are provided with Aspen Plus. The files in these folders are designed to assist in creating suitable simulation models in Aspen Plus.

4 Double-click the shortcut to the **Examples** folder, then the **GSG_Process** folder.

5 From the list of files, select **flash.bkp** and click **Open**.

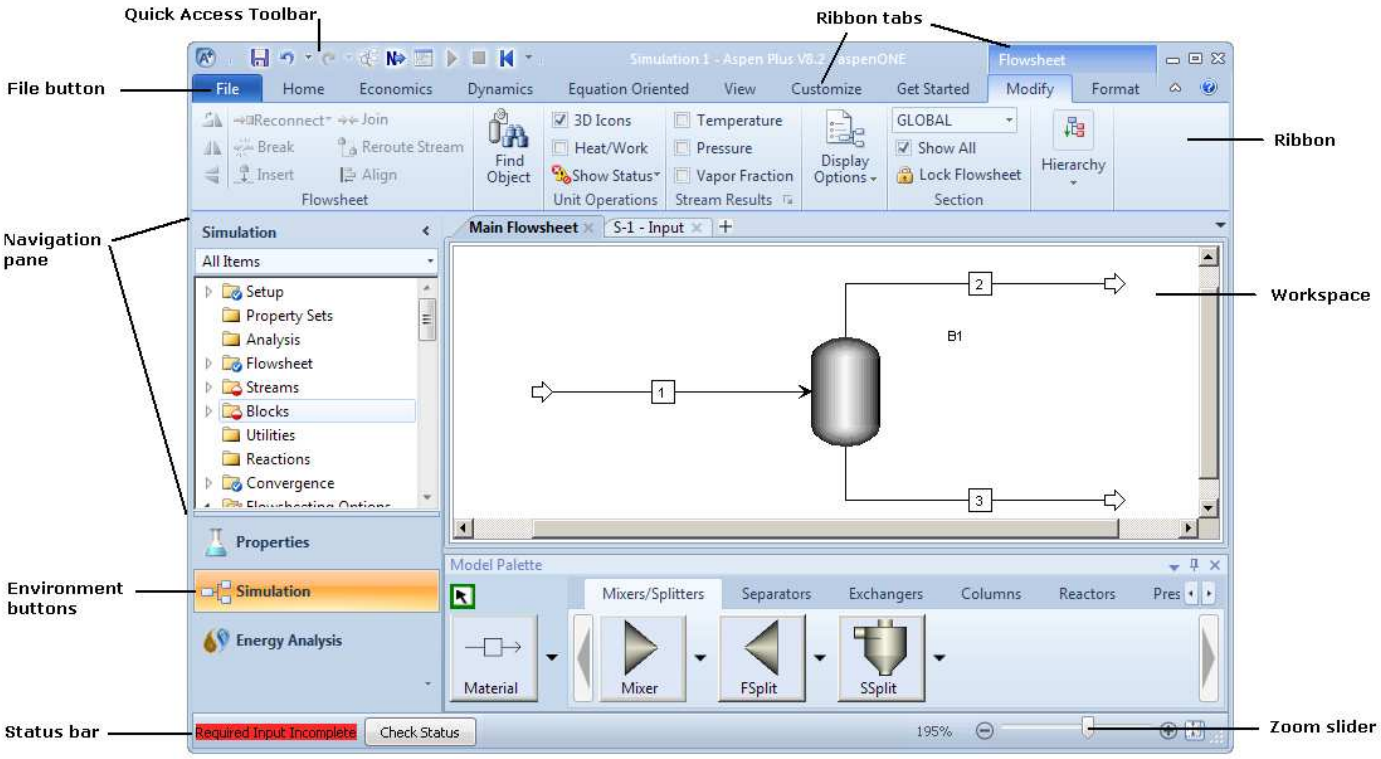
6 An Aspen Plus dialog box appears, informing you that you don't have write access to the directory containing this file, and that Aspen Plus is changing the working directory to a public one. Click **OK**.

While Aspen Plus opens the simulation model, the cursor shows the busy symbol, to indicate that Aspen Plus is finishing an operation. When the operation is complete, the cursor returns to the arrow shape.

7 Click the **Simulation** bar on the Navigation Pane to go to the Simulation environment.

The Aspen Plus Main Window

The Aspen Plus main window (shown below) appears when you start Aspen Plus. Open an Aspen Plus case, then click the **Simulation** bar on the Navigation Pane to get the display style shown below. The **Main Flowsheet** window is shown in the workspace area and the **Flowsheet** tabs appear on the ribbon along with other tabs. The Navigation Pane is on the left side of the main window to provide access to various work folders and forms.



Aspen Plus displays context-dependent definitions and information on the Messages Panel. To activate this panel, on the **View** tab of the ribbon, click **Message Panel**. Whenever you need information about the current highlighted item, refer to this area for guidance.

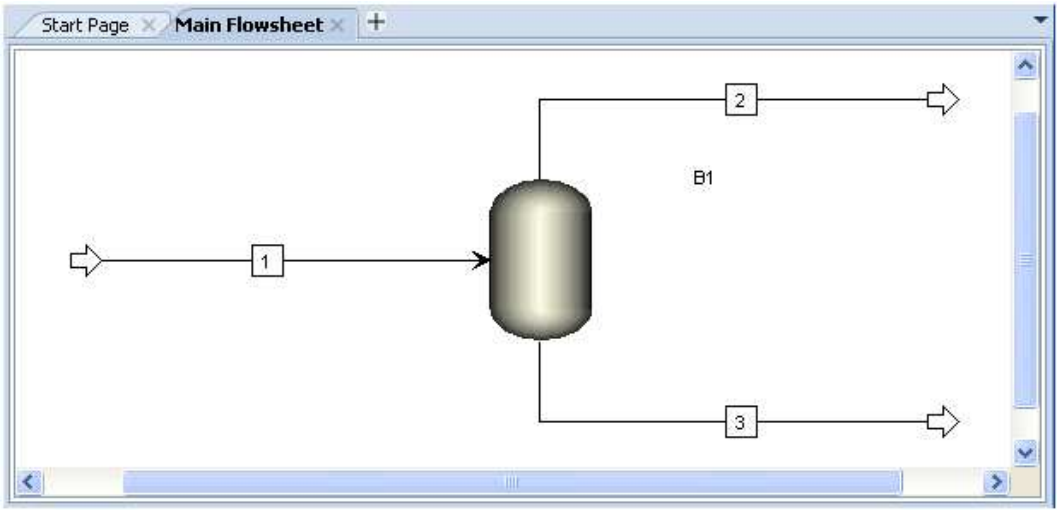
- Quick Access Toolbar — the **Quick Access Toolbar** appears at the left side of the title bar. You can customize the Quick Access Toolbar to add other frequently used commands; these commands are always visible, no matter which tab of the ribbon is active.
- Ribbon — click any of the tabs on the ribbon to access a set of related commands. These commands are split into named groups, such as **Run**, **Units**, **Summary**, **Analysis** and **Plot** on the **Home** tab.
- Navigation Pane — the Navigation Pane applies to all open forms, and updates to show the currently open form when you move to a new form or switch tabs to a previously opened one. Also, you can click the **Properties** and **Simulation** bars on the Navigation Pane to switch between the two environments.
- Tabbed windows in the workspace — forms, the flowsheet, Control Panel, plots, and other windows appear with separate tabs in the workspace. You can click and drag tabs to one side of the workspace to display them side by side, or drag them out of the Aspen Plus window entirely.
- Properties and Simulation environments — Aspen Plus is now divided into separate **Properties** and **Simulation** environments. The environment bars on the Navigation Pane let you switch between these environments.
- Status messages— the main status message (such as *Required Properties Input Complete* or *Results Available*) is shown at the bottom left side of the main window, along with the **Check Status** button, which provides

quick access to the run status and any error or warning messages from the last run.

- Zoom slider and Zoom In — use the Zoom slider and the **Zoom In** button on the right side of the Status bar to quickly adjust the size of the flowsheet, grids, plots shown in the tabbed windows in the Workspace.

Selecting Flowsheet Objects

Aspen Plus displays the process flowsheet for the opened Flash simulation:



Process flowsheets display streams and unit operation blocks. The Flash simulation has one feed stream (stream **1**), two product streams (streams **2** and **3**), and one unit operation block (**B1**).

Next, select the feed stream (stream **1**) on the process flowsheet and enter specifications.

Using a Shortcut Menu

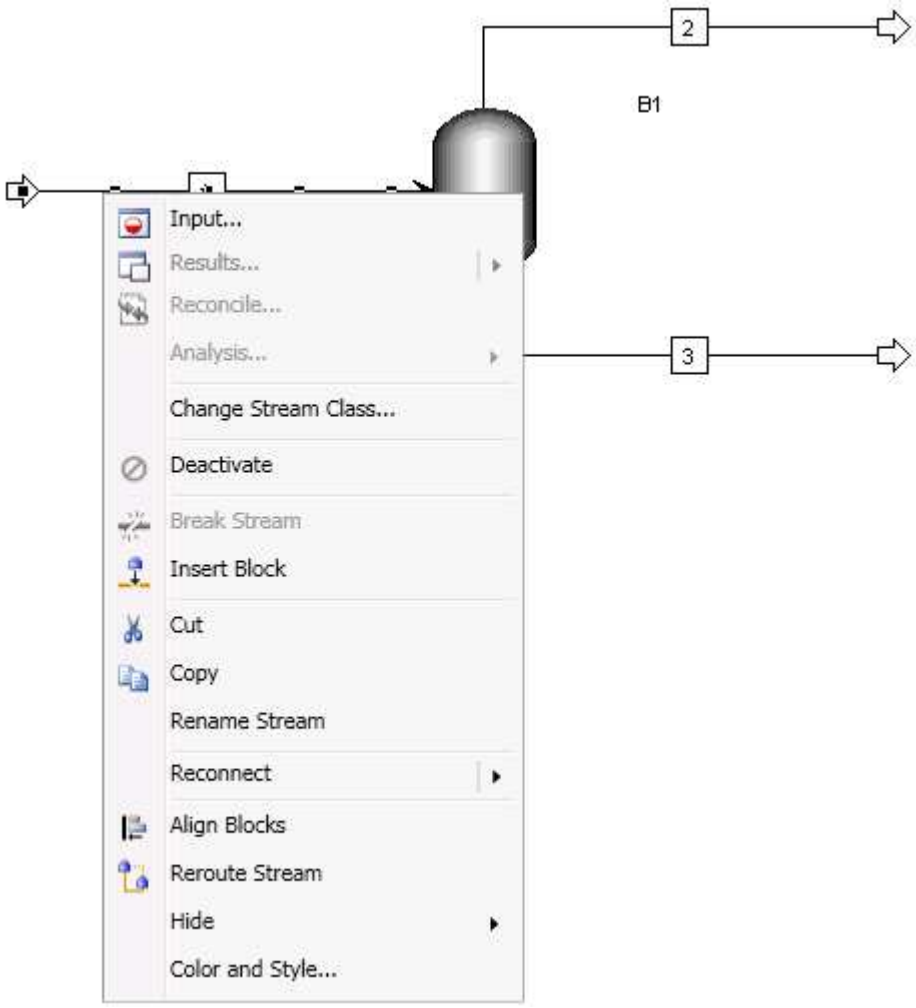
A shortcut menu of commands is available for the flowsheet objects.

To Display the Shortcut Menu for Stream 1

1 Select Stream **1** and click the right mouse button.

Note: Make sure the tip of the cursor arrow is touching the stream, otherwise you will get the flowsheet shortcut menu instead of the stream shortcut menu.

The stream shortcut menu appears, listing the executable commands for stream 1:



2 Move the cursor to highlight the commands in the shortcut menu.

Opening Input Sheets

Aspen Plus provides input sheets to allow you to specify the components of a stream and properties such as temperature. There are multiple ways to access the input sheets:

- Use the Navigation Pane to navigate to **Streams | 1 | Input** to open the **1 (MATERIAL) | Mixed** sheet.

  Note: The **item | sub-item** shorthand means "click **item** then click **sub-item**." This shorthand will be used for many hierarchical selection processes including the Navigation Pane and **File** menu.
- From the Stream **1** shortcut menu, select **Input**.

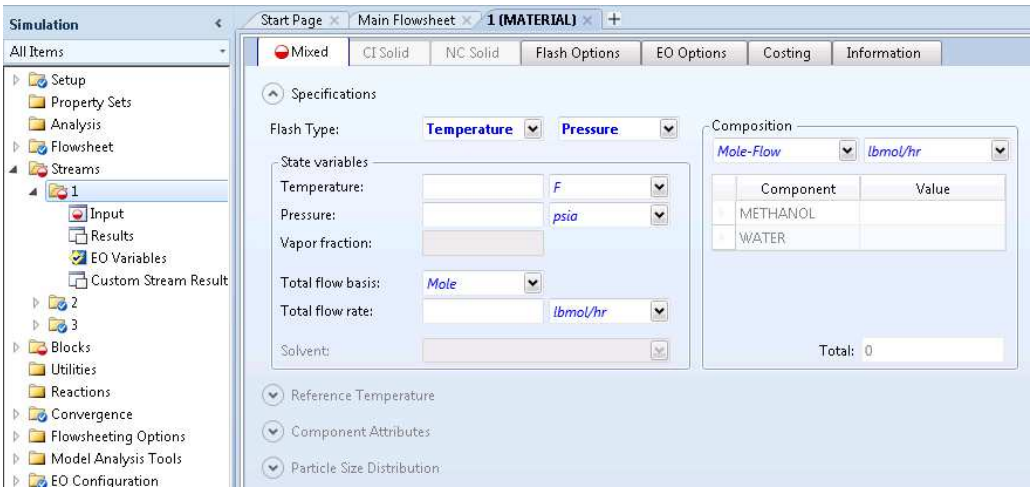
To Open the Input Sheets for Stream 1

1 From the **Main Flowsheet** window, select Stream **1**, then click the right mouse button.

2 From the stream shortcut menu, click **Input**.

Tip: To open a stream or block input sheet quickly, double-click the object from the process flowsheet.

The **1 (MATERIAL)** window appears on a separate tab in the workspace.



Note: A sheet may be required, unavailable, or optional. In this example, the **Mixed** sheet is required and incomplete (hence the symbol:). The **Flash Options**, **EO Options, Costing** and **Information** sheets are optional.

Navigate from form to form by expanding the folders in the Navigation Pane and clicking the lowest level objects. For example, if you want to see the input form for stream **1**, expand the **Streams | 1** folder by clicking the icons next to **Streams** and **1**, then click **Input**.

Navigate from sheet to sheet by clicking the large rectangular tabs at the top of the sheet. For instance, to see the **CI Solid** sheet on the **Streams | 1 | Input** form, after opening the form, click the **CI Solid** tab to the right of **Mixed**.

Navigate to other windows by clicking the window tabs in the workspace (the small tabs above the sheet tabs in the above example). For example, if you want to go back to the process flowsheet, click the **Main Flowsheet** tab to the left of **1 (MATERIAL)**.

Using Help

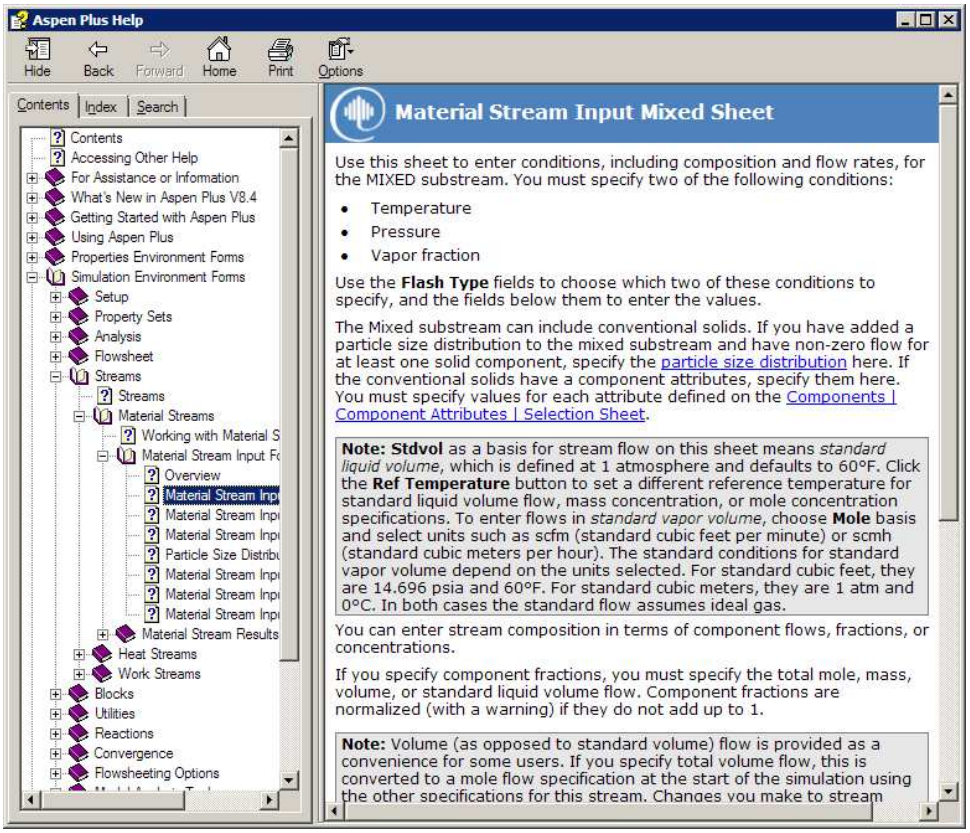
Before specifying the characteristics of Stream 1 you may wish to get context-sensitive help about the sheet itself, the form to which it belongs, or about the various fields within the sheet. To get help, click the box or sheet, then press **F1** (the help key).

Get help on the **1 (MATERIAL) | Mixed** sheet and on the whole input form.

1 Click the tab labeled **Mixed**.

2 Click **F1**.

Aspen Plus displays a help window that explains how to use the **Material Stream Input Mixed Sheet**:



3 Scroll to the end of the help topic and click the underlined text **Material Stream Input Form**.

   The **Material Stream Input Form** help topic appears.

   Aspen Plus displays the help for the Material Stream Input form, which, in this case, consists of the following sheets: **Mixed**, **CI Solid, NC Solid, Flash Options, EO Options, Costing**, **Information**.

4 When finished, close the help window.

To Get Help on any Topic

You can get help on any topic at any time by using the **Help** button.

1 At the right end of the ribbon, click 

   -or-

   press **F1** from the keyboard.

2 Use the **Up** and **Down** arrow keys on the keyboard to move through the **Help** contents.

3 In the **Contents** pane at the left, double-click **Using Aspen Plus**.

Tip: You can click **Hide** or **Show** on the help window's toolbar to hide or reveal the left pane which displays the **Contents**, **Index**, and **Search** tabs. You can click the **Index** and **Search** tabs to look for help by subject.

4 Double-click a topic labeled with the icon to display the associated help topic or double-click items labeled with the icon to view more topics.

5 When finished, close the help window.

Entering Data on a Sheet

Once an input sheet is opened, state variables, units, and numeric data may be entered into the available fields (white rectangular boxes) or selected from drop-down lists. There are two ways to move from field to field on a sheet:

- Press the **Tab** key on your keyboard.
- Position the cursor in the field and left-click.

In this simulation, enter missing temperature, pressure, and component flow data for **Stream 1**.

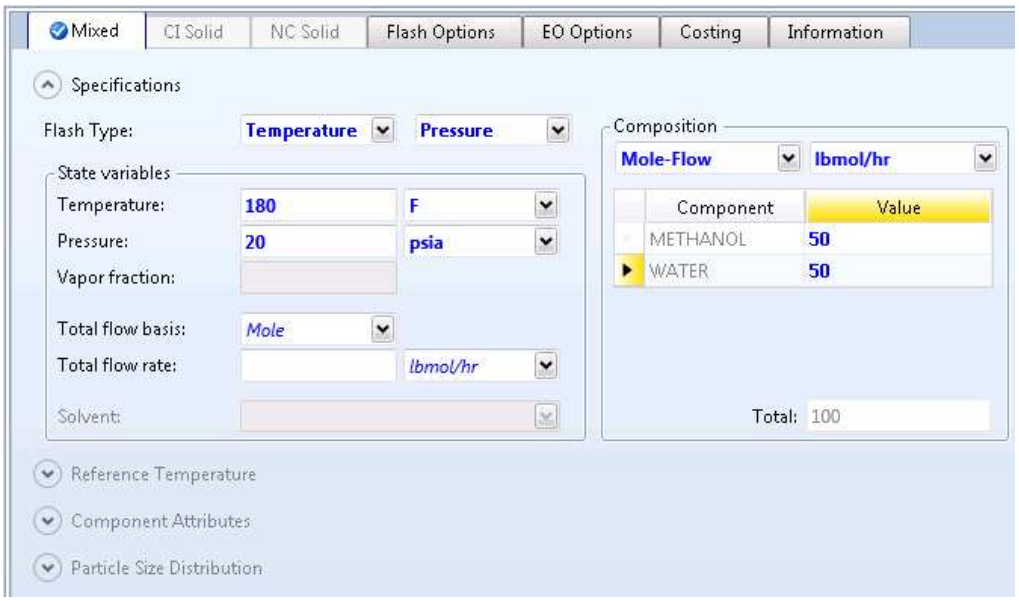
1 If necessary, click the tab for the **1 (MATERIAL)** form in the workspace to make it active.

2 Enter the following state variable and component flow specifications on the **Mixed** sheet:

Parameter	Value	Units
Temperature	180	F
Pressure	20	psia
Methanol mole-flow	50	lbmol/hr
Water mole-flow	50	lbmol/hr

Since the default units are appropriate for this simulation, you only need to enter the values.

The completed **1 (MATERIAL)** form appears below (the Navigation Pane is not shown):



When all required specifications have been entered, a check mark ( ) appears on the tab header containing the sheet name. Check marks also appear in the icons on the Navigation Pane.

Expert Guidance – the Next Function

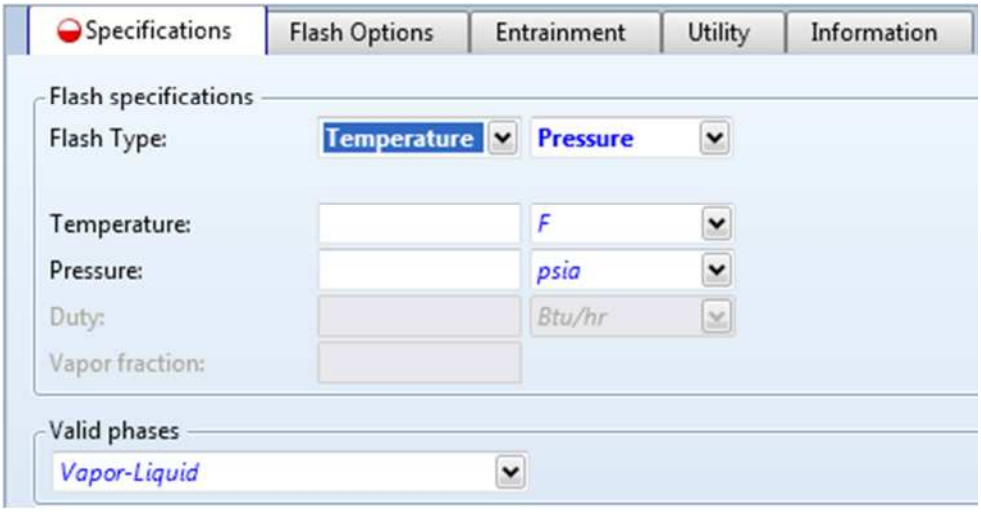
The Aspen Plus expert system, known as the **Next** function, guides you through all the steps for entering specifications for your simulation model. The **Next** function:

- Guides you through the required and optional input for a simulation by displaying the appropriate sheets.
- Displays messages informing you what you need to do next.
- Ensures that you do not enter incomplete or inconsistent specifications even when you change options and specifications you have already entered.

To Use the Next Function to Display the Next Required Form

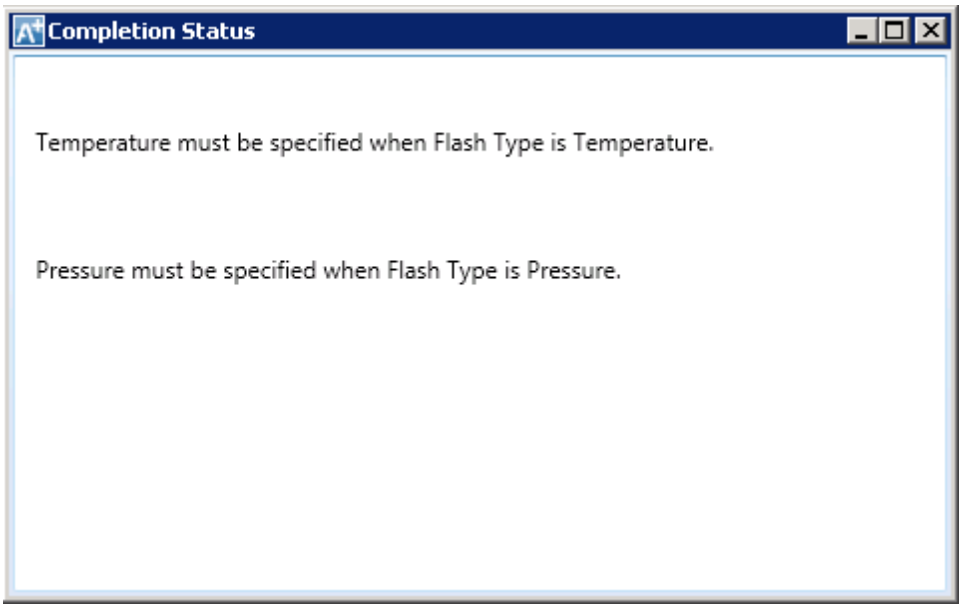
1 From the Quick Access Toolbar, click .

Aspen Plus displays the next sheet that requires input data, in this case, the **B1 (Flash2) - Input | Specifications** sheet:



Now you should enter the temperature and pressure specifications.

If you click while the sheet is incomplete, the **Completion Status** dialog box appears indicating the missing specifications:



Click **X** in the upper right corner to close the **Completion Status** message window.

2 Change the first option of **Flash Type** from **Temperature** to **Duty** by clicking and selecting **Duty** from the list. The input fields of **Pressure** and **Duty** are now active while other specifications are not valid.

This sets the necessary specification needed to run the flash calculation.

You can change the combination by clicking beside the input field for each specification, and then selecting other options from the list.

3 In the **Pressure** value field, type **1**.

4 In the **Pressure** units field, click and select **atm** to change the input units from psia to atm.

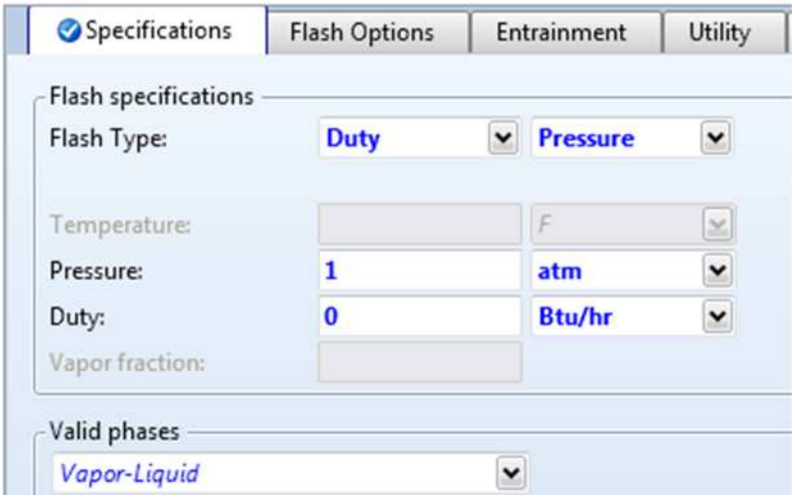
5 In the **Duty** value field, type **0**.

There is no need to change the units (**Btu/hr** is the default).

6 The box in the **Valid phases** area is set to **Vapor-Liquid** by default. For this simulation, accept the default.

Note: Default values on input sheets appear in blue and italic unless you modify them, in which case they will appear in blue and bold text.

The input data on the **B1 (Flash2) - Input** form is now complete:



The check marks ( ) on the Navigation Pane and the absence of partially filled circles ( ) indicates that all required data have been entered on forms. The **Required Input Complete** message at the lower left corner of the main window indicates that all required data in the entire model have been entered.

Running the Simulation

The input specifications for this simulation model are complete and the simulation is ready to be run. Run the simulation in either of the following ways:

- From the **Home** tab of the ribbon, in **Run**, click .
- From the Quick Access Toolbar, click .
- Press **F5**.

Once the process flowsheet has been fully specified, running the simulation is easy.

To Run the Simulation

On the **Home** tab of the ribbon, in **Run**, click .

While Aspen Plus performs calculations for the simulation, the cursor has a stop sign shape. The block being executed is also highlighted in the process flowsheet window. When the calculations are complete, the cursor returns to the arrow shape. On the Status bar at the bottom of the main window, the message *Results Available* appears on the left.

The **Economic Analysis** dialog box appears. If you want to evaluate the capital and operating costs, make sure that you have installed and have a valid license for Aspen Process Economic Analyzer before clicking **Activate**.

Note: Click **Control Panel** in **Run** to open the Control Panel and check the run-time message for the calculation. If the calculation completes with errors or warnings, the warning or error messages will be shown on the Control Panel.

Examining Stream and Block Results

Now view the results for the flash overhead vapor stream (Stream 2) and for the flash block (Block B1).

To Display the Flash Overhead Vapor (Stream 2) Results

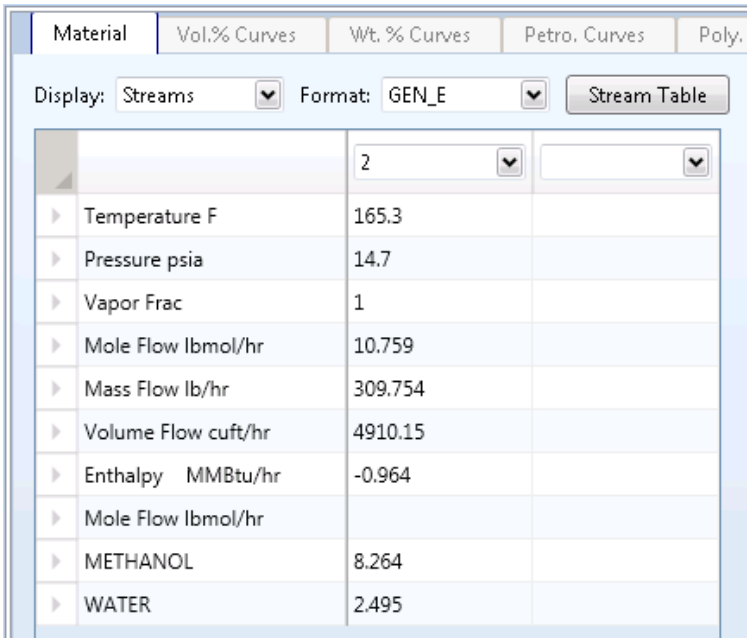
1 Display the process flowsheet by clicking the **Main Flowsheet** tab in the workspace.

Note: If the streams in your process flowsheet now have temperature and pressure data attached to them, you can remove these attachments by clearing the check boxes for **Temperature** and **Pressure** in **Stream Results** on the **Flowsheet | Modify** tab on the ribbon. After that, you may wish to click the **View** tab on the ribbon, in **Zoom,** select **Zoom Out** or **Zoom to Fit** to make your flowsheet look nice with the attachments.

2 Select stream **2** and right-click on the stream to display the shortcut menu.

3 From the shortcut menu, select **Results**.

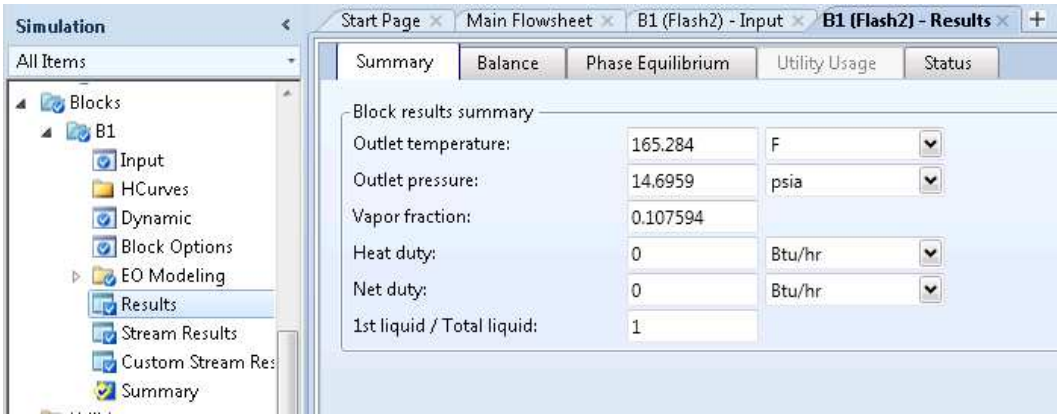
The **2 (MATERIAL) - Results** form opens in a new window tab, providing the thermodynamic state and composition flows of the vapor stream:



4 From the Navigation Pane, select **Blocks | B1 | Results**.

Note: You can expand the tree items shown on the Navigation Pane by clicking the ▷ symbol next to a closed folder. When you select a new folder, it automatically expands with the first item selected.

The **B1 (Flash2) - Results** form appears with the overall results for the block:



5 Review the calculated flash outlet temperature and overall vapor fraction.

6 Click each tab shown in the **B1 (Flash2) - Results** window to browse through the results. For example, click the **Balance** tab to review the mass and energy balance data, and **Phase Equilibrium** tab to review the vapor-liquid equilibrium results.

Modifying and Rerunning Your Model

1 From the process flowsheet, select and right-click stream **1** to display the stream shortcut menu.

2 Select **Input**.

The **1 (MATERIAL)** form opens in a new window tab, with data on the **Mixed** tab displayed in view.

3 In the **Composition** area, enter the following values for the component mole-flows:

Component	Value
Methanol	60
Water	40

On the Navigation Pane, the icons in front of the folder and form names have changed to  and  , indicating the input data changed in these forms.

4 On the **Home** tab of the ribbon, in **Run**, click  to run the simulation with the new feed stream values.

5 When the run is completed, display the new results for the outlet streams and the flash block.

Saving Your File and Exiting Aspen Plus

For this example, save your file as both an Aspen Plus document (.apw) file and an Aspen Plus backup (.bkp) file. Document files contain all the intermediate convergence information from the simulation and are useful for saving long simulations. This information is *not* forward compatible for new versions of Aspen Plus. When you open a Document file in a newer version of Aspen Plus, a backup file embedded in that document file will be used, instead.

Backup files are compact, portable, and are forward compatible but contain only the input specifications and simulation results. The first run using a backup file will take just as long as the very first run of the simulation.

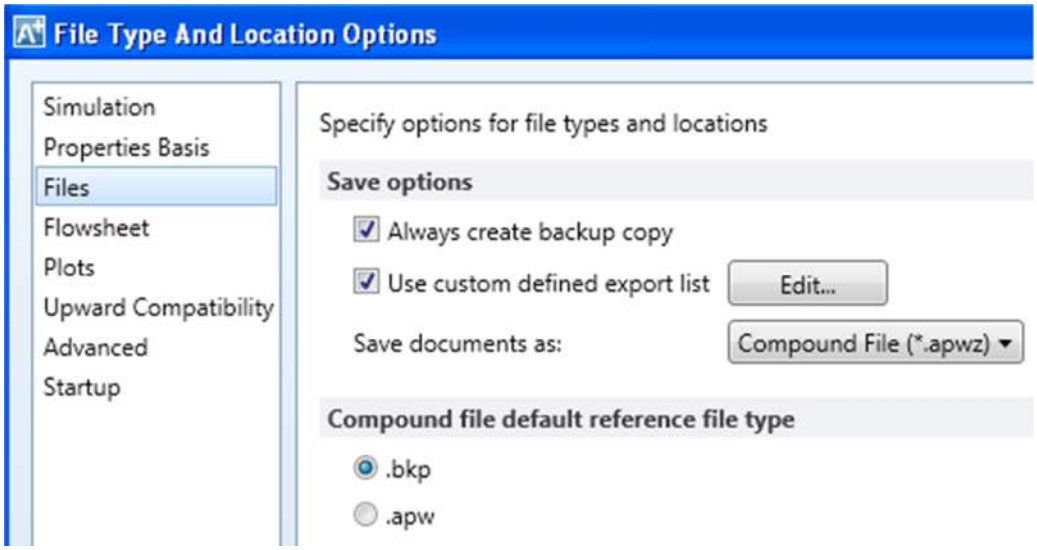
First, set Aspen Plus to create a backup file with each save.

To Change the Save Options

1 On the upper left corner of the ribbon, click **File** to open the **File** menu. Click **Options** at the bottom of the menu.

The **Simulation Run Options** dialog box appears.

2 In the left pane, click **Files** to display the options available for file settings.



3 In the **Save options** area, select the check box next to **Always create backup copy**, if it is not already checked.

4 Click **OK**.

Next, save the simulation and exit Aspen Plus.

To Save and Exit

1. On the ribbon, click **File** and then move your cursor to **Save As**. A list of available file types appears on the right side of the menu.
2. Click **Aspen Plus Document** to save your simulation as an Aspen Plus document (.apw) file. The **Save As** dialog box appears.

   If necessary, use the **Save in** list to navigate to your Aspen Plus working folder. In this example, the folder is located in <driver>:\Program Files\AspenTech\Working Folders\Aspen Plus <version>.
3. Type **Flash** as the file name in the **File name** field. Click **Save**.

   Aspen Plus will place a file called **Flash.apw** and a file called **Flash.bkp** in your Aspen Plus working folder. See the *Aspen Plus User Guide* for detailed descriptions of the characteristics of these files.
4. On the ribbon, click **File** and select **Exit.**

You have completed an Aspen Plus simulation.

2 Building and Running a Process Simulation Model

In this simulation, create an Aspen Plus process model for a methylcyclohexane (MCH) recovery column.

This simulation is divided into three sections:

1 Building the Process Model.

2 Adding Data to the Process Model.

3 Running the Simulation.

4 Examining the Results.

Allow about 50 minutes for this simulation.

Building the Process Model

In this section, build the process model by performing these tasks:

1 Define the process to be simulated.

2 Start Aspen Plus.

3 Create a new simulation.

4 Define the required properties.

5 Build a process flowsheet.

Defining the Simulation: Methylcyclohexane Recovery Column

The process flow diagram and operating conditions are shown in Figure 2.1

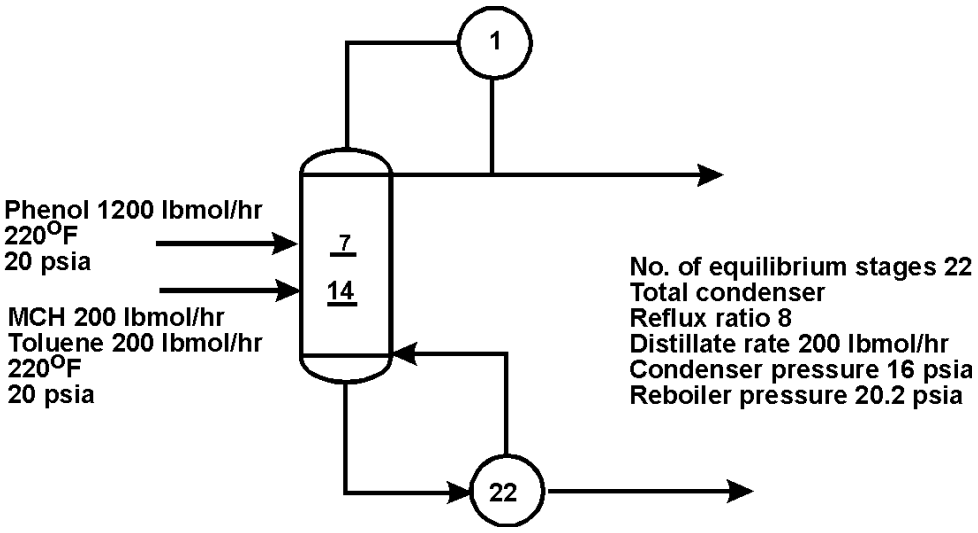


Figure 2.1 Simulation Definition: MCH Recovery Column

MCH and toluene form a close-boiling system that is difficult to separate by simple binary distillation. In the recovery column in Figure 2.1, phenol is used to extract toluene, allowing relatively pure methylcyclohexane to be recovered in the overhead.

The purity of the recovered methylcylohexane depends on the phenol input flow rate. In this session, create an Aspen Plus simulation that allows you to investigate the performance of the column.

Starting Aspen Plus

1 From your desktop, select **Start** and then select **Programs**.

2 Select **AspenTech,** then **Process Modeling <version>,** then **Aspen Plus**, then **Aspen Plus <version>.**

The **Aspen Plus** main window appears, showing the **Start Using Aspen Plus** window.

For more information about this window, see "**The Aspen Plus Main Window**" on page 9.

Create a new simulation using an Aspen Plus built-in template.

Creating a New Simulation

Aspen Plus provides built-in templates for applications such as chemicals, petroleum, electrolytes, specialty chemicals, pharmaceuticals, and metallurgy.

1 On the ribbon, click **File** and select **New**.

The **New** dialog box appears. Use the **New** dialog box to choose an appropriate template for the new run.

To Specify the Template for the New Run

2 From the pane on the left of the **New** dialog box, click **Chemical Processes** so that the chemical processes templates are shown.

3 Click the **Chemicals with English Units** template.

4 Click **Create**.

It takes a few seconds for Aspen Plus to finish setting up the new problem.

The template is loaded with default settings for the simulation.

Defining the Required Properties

Aspen Plus provides three working environments, **Properties**, **Simulation**, and **Energy Analysis**. The **Properties** environment includes the set of features available in Aspen Properties. For more information about Aspen Properties, please refer to *Aspen Properties Help*. In the **Simulation** environment, you can work on the process flowsheet, specify process data, and execute the calculation. It is recommended that you set up all required properties settings before configuring the simulation. The **Energy Analysis** environment is used for optimizing energy usage in a completed simulation model, and will not be covered in this document.

Note: Switch between the environments by clicking the **Properties** and **Simulation** bars on the Navigation Pane. The list of folders and forms on the Navigation Pane varies in different environments, and the available ribbon tabs and the open windows also differ among the environments. For example, the **Main Flowsheet** window can only be opened in the Simulation environment; as a result, the **Flowsheet** tabs only appear on the ribbon when you are in the Simulation environment and looking at the Flowsheet window.

Aspen Plus starts a new simulation from the Properties environment. If you need to specify the process flowsheet first, click the **Simulation** bar on the Navigation Pane to switch to the Simulation environment.

Entering Components

Use the **Components - Specifications** form in the **Properties** environment to select the chemical components present in the simulation.

1 Check if you are in the Properties environment by looking at the bars on the Navigation Pane. The **Properties** bar should be highlighted, indicating that the current environment is **Properties**.

2 From the Navigation Pane, click **Components | Specification** to open the form.

The components for the process in this simulation are toluene, phenol, and methylcyclohexane.

To Enter a Unique Component ID for Each Component

1 In the **Component ID** field, type **TOLUENE** and press **Enter** on the keyboard.

Because Aspen Plus recognizes the component name Toluene as an Aspen Plus databank component, it fills in the **Type, Component name,** and **Alias** fields automatically.

2 In the next **Component ID** field, type **PHENOL** and press **Enter** on the keyboard.

Note: If the **Update Parameters** dialog box appears, click **Yes** to continue.

Aspen Plus again fills in the remaining fields.

3 In the next **Component ID** field, type **MCH** and press **Enter** on the keyboard.

The Aspen Plus databank does not recognize the abbreviation MCH.

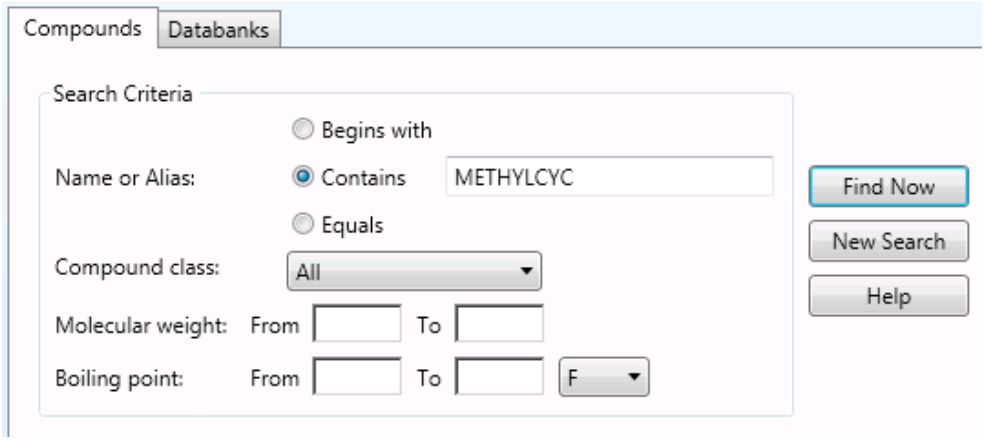
4 In the **MCH** component name row, type **METHYLCYC** in the **Component name** field and press **Enter** on the keyboard.

The **Find Compounds** dialog box appears.

5 Click the **Databanks** tab and the click 

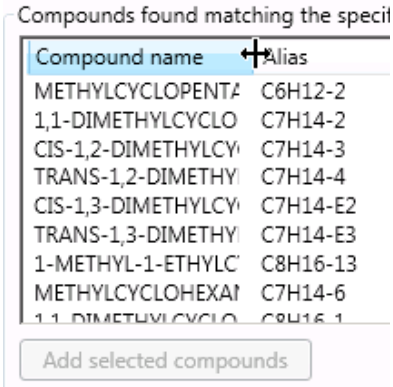
to move all to the Selected databanks list.

6 Click the **Compounds** tab, select **All** for **Compound class**.

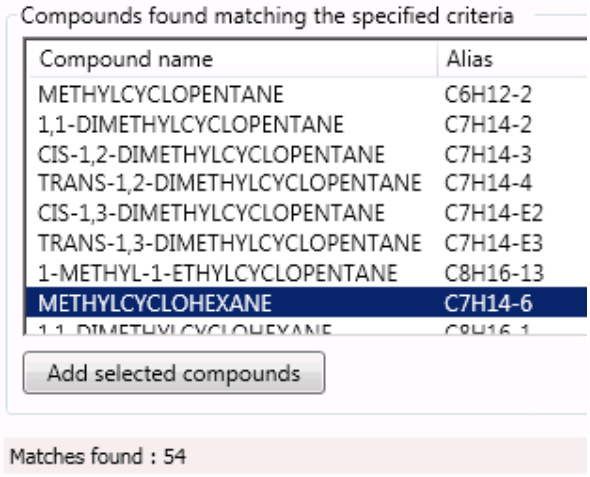


7 Click **Find now** to list all the components in the Aspen Plus databank that have a name containing METHYLCYC.

8 The resulting compound names are very long. To view the whole names, move the cursor to the right edge of the Compound name column, until it turns into the ✣ shape, then click and drag to the right.



9 From the list of components found from the databanks, locate and select **METHYLCYCLOHEXANE**.

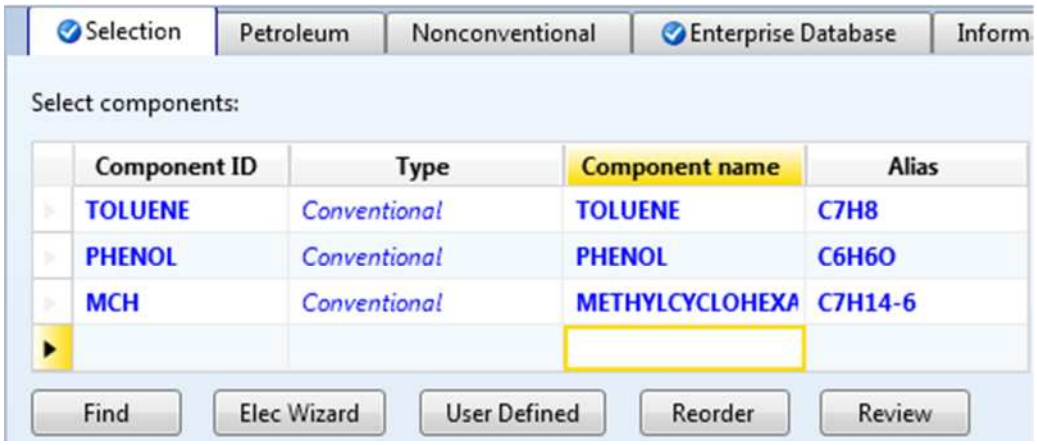


10 Click **Add selected compounds**.

11 Click **Close**.

Note: If you need to search for components based on molecular weight range, boiling point range, or CAS numbers, specify values in the fields on the **Compounds** tab to perform advanced search.

You have now specified the three components required for this process simulation model: Toluene, Phenol, and Methylcyclohexane:



12 Click .

Note: You can navigate to the incomplete forms yourself by clicking on folders in the tree view on the Navigation Pane marked with the symbol.

The **Binary Interaction -NRTL-1 (T-DEPENDENT) | Input** sheet appears.

13 From the Navigation Pane, click **Methods | Specifications**.

Methods - Specifications | Global sheet appears. This sheet is already complete with the default settings from the Chemicals with English Units template.

Selecting Thermodynamic Methods

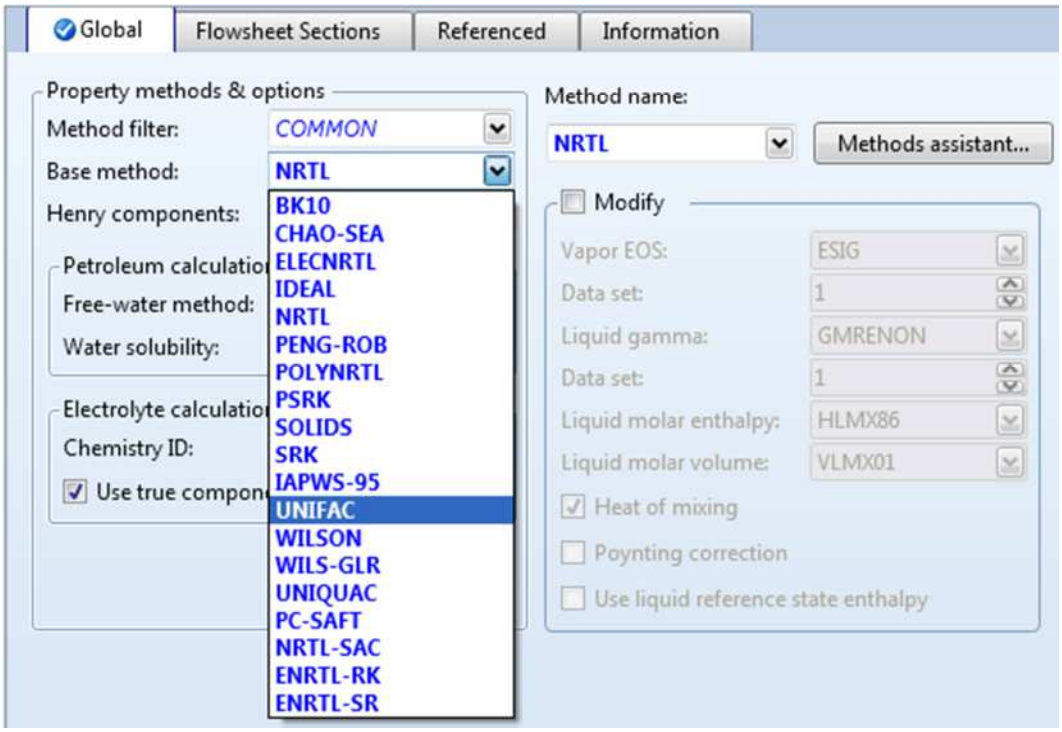
Use the **Methods - Specifications** form to select the property method used to calculate properties such as K-values, enthalpy, and density. The **Base method** list contains various property methods built into Aspen Plus. The specific methods in the list depend on the chosen method. To see all the available methods (a very long list), in the **Method filter** field, click and select **ALL**.

Note: Clicking the **Modify** check box allows you to create a custom property method that starts out identical to the chosen base method but may be modified according to your needs. For more information, see the online help topic **Using Aspen Plus | Entering Property Specifications | Physical Property Methods**.

For this simulation, use the **UNIFAC** property method to calculate thermodynamic properties.

To Find the Appropriate Type of Base Method for this Simulation

1 In the **Base method** list, click to display the available property methods in Aspen Plus:



Get a brief description of a base method by selecting it and reading the messages shown in the **Messages Panel**. For detailed information about a base method, refer to the *Physical Property Methods* reference manual.

2 From the **Base method** list, select **UNIFAC**.

3 Click .

The **Properties Input Complete** dialog box appears.

The *Required Properties Input Complete* message appears on the left side of the Status bar.

Aspen Plus can run the properties calculation if you select the **Run properties analysis / setup** option in the **Required Properties Input Complete** dialog box.

4 Select the option **Go to Simulation environment** and click **OK**.

You have completed the required input for properties.

Now enter the **Simulation** environment to build the process flowsheet and input the process data.

The process flowsheet window now opens in a window named **Main Flowsheet**. It docks in the workspace (beside other open windows, if any).

Defining the Flowsheet

In the flowsheet for the MCH process shown in Figure 2.1, there are two feed streams (MCH-toluene feed and phenol solvent), one unit operation (an extractive distillation column), and two product streams (distillate and bottoms).

Set up the Aspen Plus process flowsheet by placing the unit operation block in the workspace and connecting four streams to it.

If you do not see the **Model Palette** below the Flowsheet:

To Open the Model Palette

1 Click the **View** tab on the ribbon.

2 Click **Model Palette**.

The Model Palette docks below the Flowsheet with icons for the unit operation blocks shown on several tabs.

To Select a Unit Operation Block

1 On the Model Palette, click the **Columns** tab.

The list of available distillation columns appears displayed as a row of icons. Moving the cursor over a block causes a description to appear beside the block icon.

2 Read the prompt for the **RadFrac** block.

The description suggests this is the right model for this simulation.

3 Select **RadFrac,** then press **F1** (the Help key) on the keyboard.

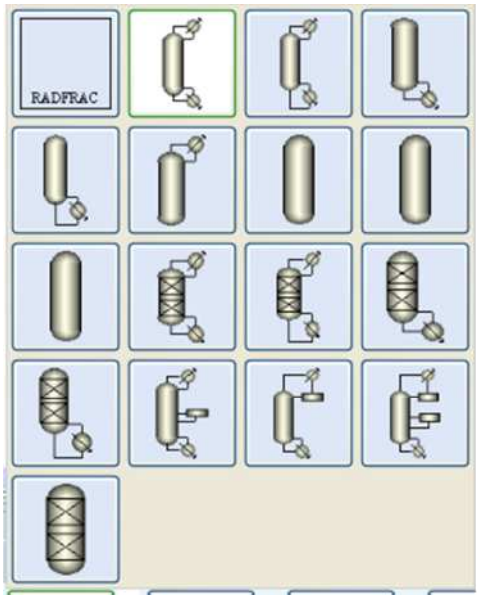
The help information confirms that **RadFrac** is suitable for extractive distillation.

4 Close the Help window.

A number of icons are available to represent the **RadFrac** block.

To Choose a RadFrac Icon and Place a Block

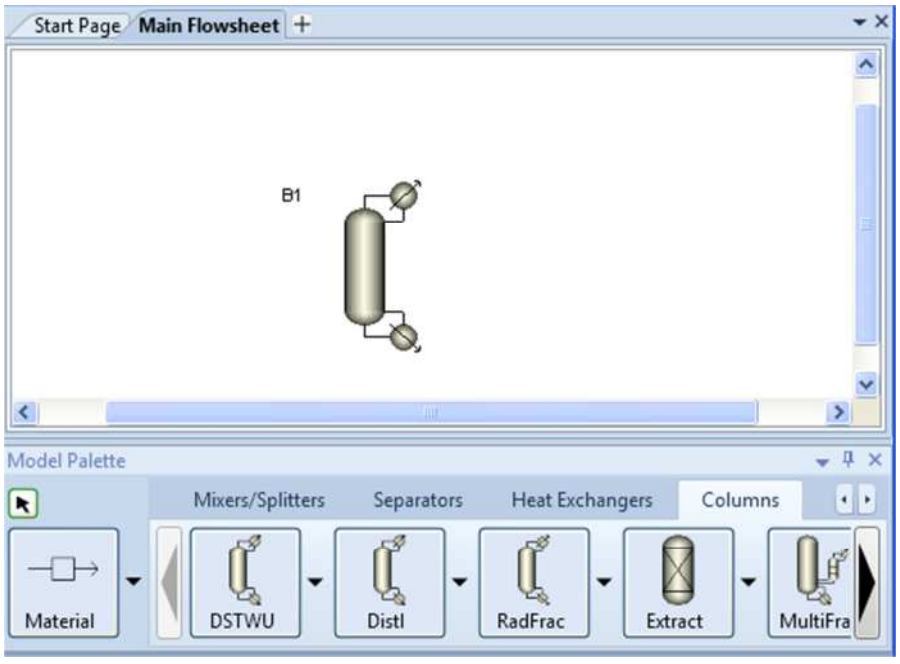
1 Click the arrow to the right of the **RadFrac** column.
The available icons for **RadFrac** appear:



2 Move the cursor over the displayed icons to view the label for each icon.

3 Click the icon labeled **FRACT1** to select the model.

4 Move the mouse to the middle of the workspace and click the left mouse button.
The block appears on the flowsheet with the default name **B1**:



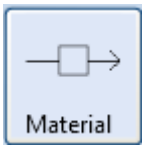
5 To stop the automatic naming of blocks and streams, on the **Modify** tab of the ribbon, click the arrow at the bottom right corner of **Stream**

Results, this opens the **Flowsheet Display Options** dialog box. Clear the check boxes in front of **Automatically assign block name with prefix** and **Automatically assign stream name with prefix**. Click **Apply** and then **OK** to close the dialog box.

Notes about block placement:

- **FRACT1** is now the default icon for the **RadFrac** block.
- Clicking once on an icon enables multiple block placement. The cursor becomes a crosshair and you can click anywhere on the process flowsheet to place any number of blocks. Click  or the right mouse button when finished.
- Your RadFrac block may have a 3-D appearance. The **3D Icons** check box in **Unit Operations**, on the **Modify** tab of the ribbon determines whether these icons are used.

To Connect Streams to the Block

1 From the Model Palette, click 

once. This will allow you to place multiple streams.

2 Move the cursor (now a crosshair) onto the process flowsheet.

Ports on the block that are compatible with the stream are indicated by arrows. Red means required; blue means optional. Hover over a port to see a description.

3 Find the **Feed (Required; one or more)** port and click once to connect a feed stream to the port.

4 Move the cursor to any blank part of the process flowsheet and click once to begin the feed stream at that location. The **Add Stream** dialog box appears. Type **1** as the name for the feed stream.

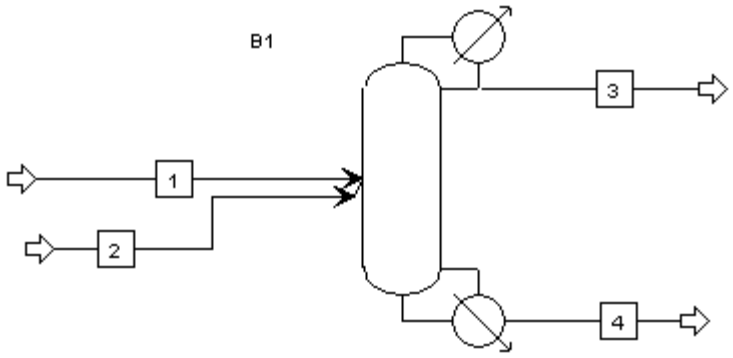
5 Create another material feed stream, stream **2**, connecting to block **B1** at the same port as Stream 1 by repeating steps 3 and 4.

6 Create another stream (Stream **3**) connected to the liquid distillate port near the top of the block. The full name of this port is: **Liquid Distillate (Required if Distillate Vapor Fraction < 1 (Setup Condenser sheet)).**

7 Connect Stream **4** to the **Bottoms (Required)** port.

8 Click  to stop adding streams.

Your process flowsheet is now complete:



The status indicator in the bottom left corner of the main window says *Required Input Incomplete* indicating that further input specifications are required before running the simulation.

Notes about Stream placement:

- To select a Heat or Work stream instead of a Material stream, click the arrow next to the stream icon on the left side of the Model Palette and choose either the **Heat** or **Work** stream icon.
- To cancel connecting a stream at any time, press the **Esc** key on the keyboard or click the right mouse button.
- You can delete a stream by selecting it and pressing the **Delete** key. However, Aspen Plus will continue to increment the numeric label for new streams, if they are being labeled automatically.
- To rename a particular stream, select it, right-click, and click **Rename Stream** on the shortcut menu.
- The easiest way to get the shortcut menu is to select the stream label and right-click in its box.
- Click the stream icon on the Model Palette and drag to place a single stream. Drag to a port and release the left mouse button to connect the stream. Move the cursor to any blank area or another port and click once to place the other end of the stream.

Adding Data to the Process Model

Now that you have created your process flowsheet, use the input forms to enter the remaining required information for this run.

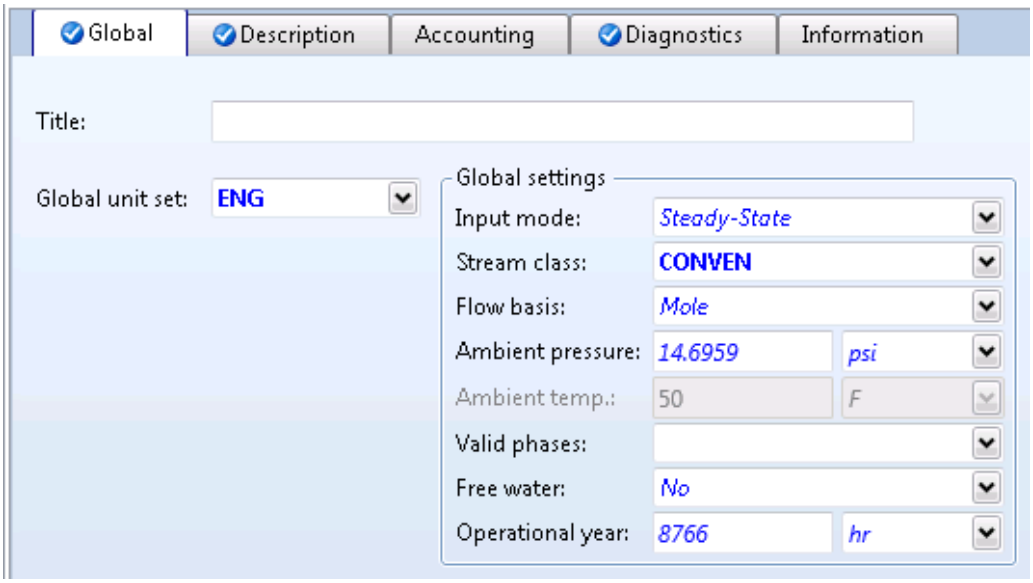
The Aspen Plus **Next** function (available with the button in the Quick Access Toolbar and Home tab of the ribbon) displays the required input sheets automatically. You can also navigate to an input sheet in any of the following ways:

- Use the Navigation Pane to navigate to any input form.
- Select a stream or block in the process flowsheet, right-click, and then select **Input** on the shortcut menu.
- Double-click a stream or block in the process flowsheet.

Specifying a Title for the Simulation

1 From the Navigation Pane, click **Setup | Specifications**.

The **Setup - Specifications | Global** sheet appears.



2 In the **Title** box, enter the text **Methylcyclohexane Recovery Process** and press **Enter** on the keyboard.

The **Setup - Specifications** form displays a number of settings that apply to the whole simulation. The chosen template set the units to English (**ENG**). These may be changed here globally, or in other sheets for particular streams or blocks. For more information about global specifications, see the online help topic **Using Aspen Plus | Entering Data for Simulations | Global Information for Calculations**.

Specifying Data to be Reported

Results data may be examined interactively in Aspen Plus or after exiting by viewing a report file with a text editor.

For this simulation, tell Aspen Plus to calculate mole fractions as well as a built-in set of properties called **TXPORT**.

1 Navigate to **Setup | Report Options** by clicking once on the **Report Options** form under the **Setup** folder on the Navigation Pane.

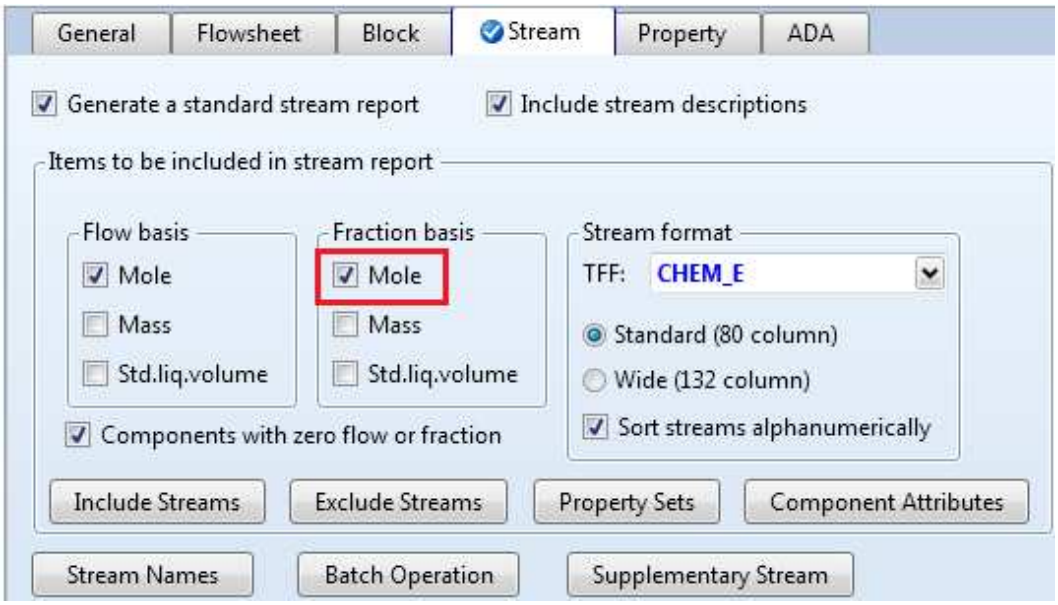
Note: If the **Report Options** form is not visible click the ▷ symbol next to the **Setup** folder to expand it.

The **Setup - Report Options | General** sheet appears.

By clicking the appropriate tab, you can customize the reporting for specific parts of the simulation.

2 Click the **Stream** tab.

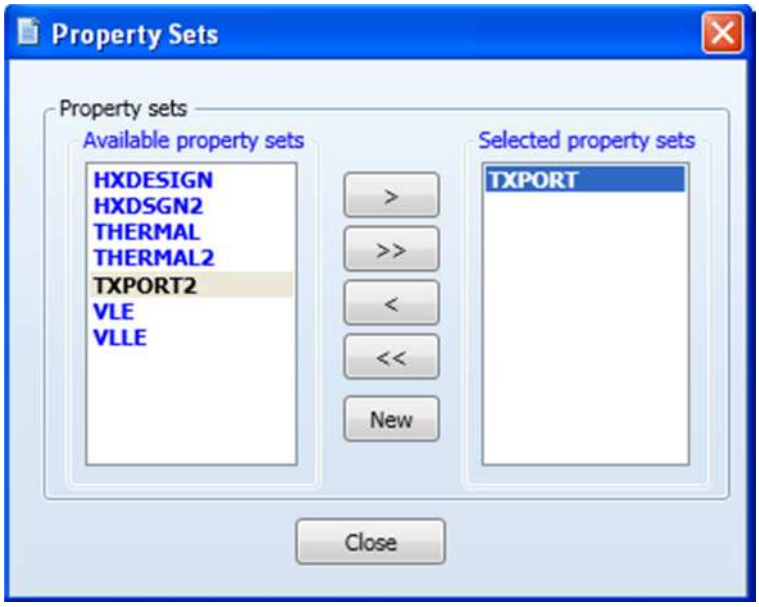
3 In the **Fraction basis** area, select the **Mole** check box.



Now Aspen Plus will calculate and report mole fractions of all stream components.

4 Click **Property Sets**.

5 The template you chose at startup contains a number of available property sets. Select **TXPORT** from the list and click > to move the property set to the **Selected property sets** column.



Now Aspen Plus will calculate and report density, viscosity, and surface tension for all streams. To learn more about Aspen Plus built in property sets and user-defined property sets, see the online help topics **Using Aspen Plus | Entering Data for Simulations | Global Information for Calculations | Report Options | Customizing the Stream Report**

| Designating Property Sets and **Aspen Plus Reference | Physical Property Data Reference Manual | Property Sets**.

6 Click **Close**.

7 Click .

The **1 (MATERIAL) - Input** form appears.

Entering Stream Data

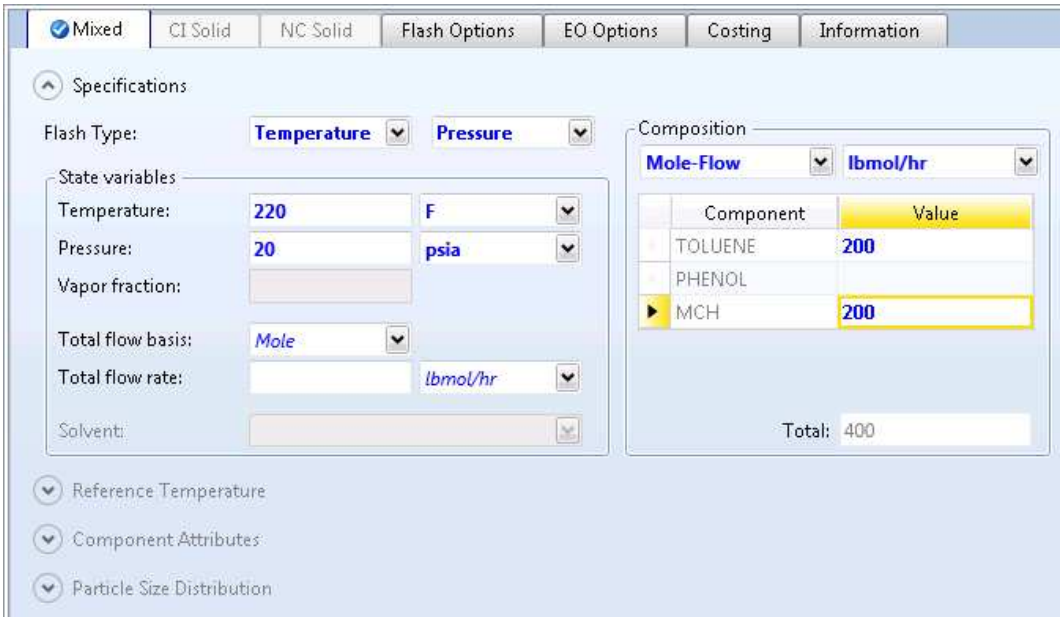
Make Stream 1 the MCH-Toluene feed stream.

1 On the **1 (MATERIAL) - Input | Mixed** sheet, enter the following state variable and component flow specifications for the MCH-Toluene feed stream:

Parameter	Value	Units
Temperature	220	F
Pressure	20	psia
Toluene flow rate	200	lbmol/hr
MCH flow rate	200	lbmol/hr

Because the default parameters and units are correct for this simulation, you only need to enter the values.

The **1 (MATERIAL) - Input | Mixed** sheet is complete:



2 Click .

The **2 (MATERIAL) - Input | Mixed** sheet appears.

Make Stream 2 the phenol feed stream.

3 Enter the following specifications for Stream 2:

Parameter	Value	Units
Temperature	220	F
Pressure	20	psia
Phenol flow rate	1200	lbmol/hr

4 Click .

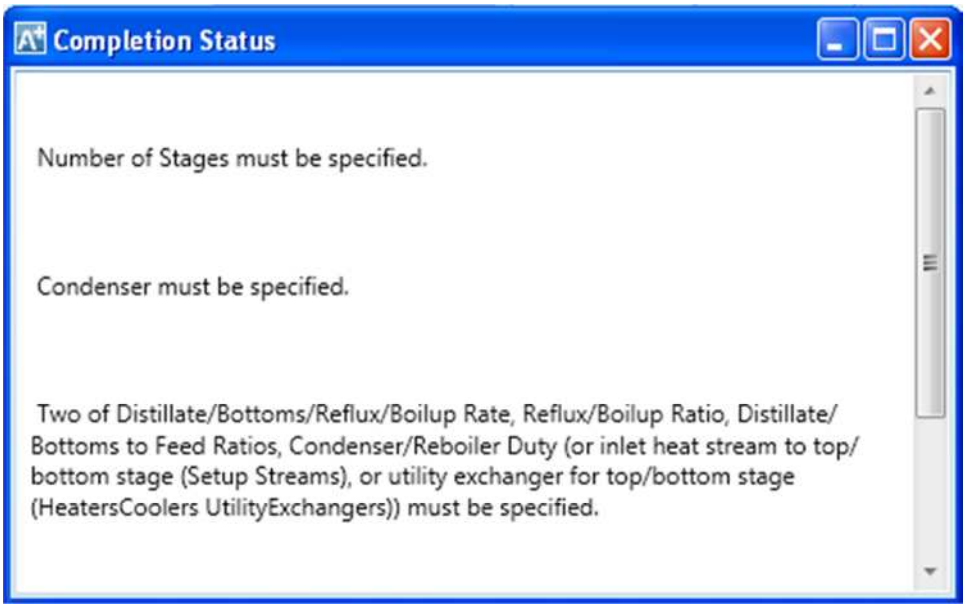
The **B1 Specifications - Setup | Configuration** sheet appears:

Entering Unit Operation Block Data

On the **B1 (RadFrac) - Setup** form, the number of stages, the condenser type, and two operating specifications are required data. The reboiler type, valid phases, and convergence method have default choices displayed in shaded type.

1 Click each box and read the descriptive messages on the Message Panel. To view the Message Panel, on the **View** tab of the ribbon, click **Message Panel**.

If you click while the sheet is incomplete, the **Completion Status** message box appears indicating the missing specifications:



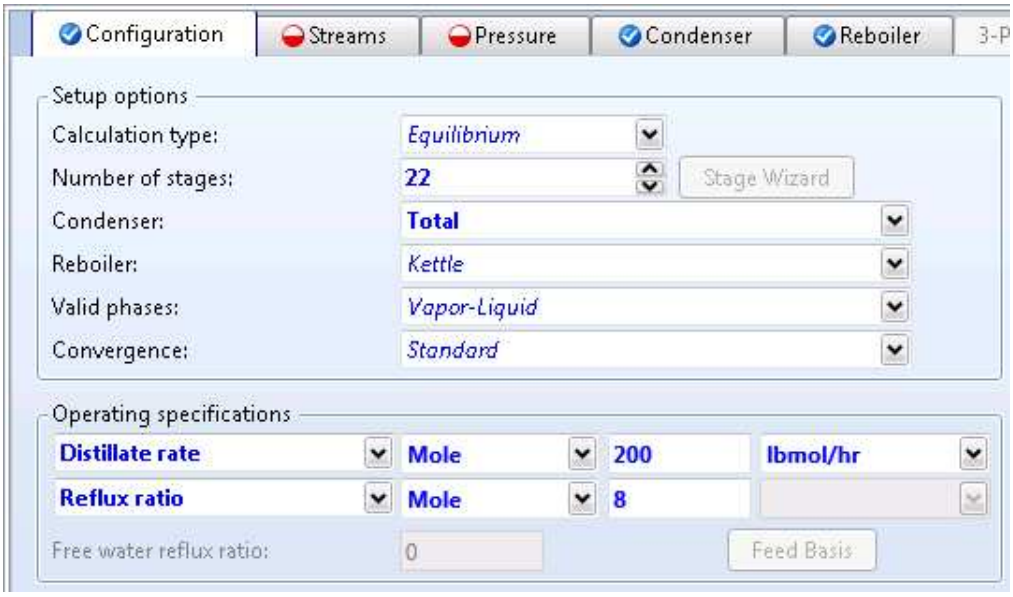
Close the **Completion Status** dialog box.

2 Enter the following specifications for the column:

Parameter	Value	Units
Number of stages	22	—
Condenser	Total	—
Distillate rate	200	lbmol/hr
Reflux ratio	8	—

Accept the defaults in the **Reboiler**, **Valid phases**, and **Convergence** fields.

The blue check mark on the **Configuration** tab indicates the sheet is complete:



3 Click or click the **Streams** tab.

The **B1 (RadFrac) - Setup | Streams** sheet appears.

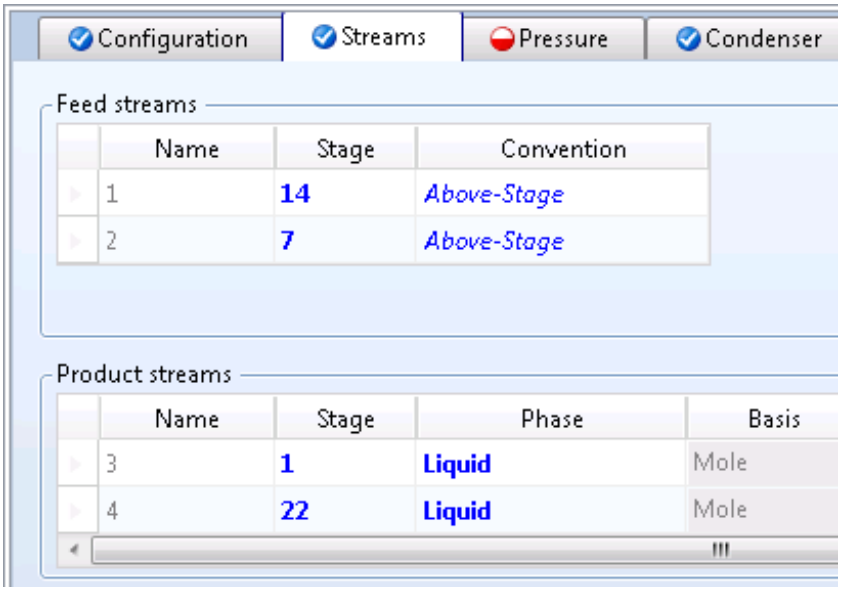
In the RadFrac model, there are N stages. Stage 1 is the top stage (the condenser); stage N is the bottom stage (the reboiler). As shown in Figure 2.1, the MCH-Toluene feed (stream 1) enters above stage 14, and the phenol solvent stream (stream 2) enters above stage 7.

4 Enter **14** in the **Stage** field for Stream 1.

5 Enter **7** in the **Stage** field for Stream 2.

6 Accept the defaults for the entry point conventions for the feed streams and for the locations and phases of the product streams.

The **B1 (RadFrac) - Setup | Streams** sheet is complete:



7 Click .

The **B1 (RadFrac) - Setup | Pressure** sheet appears.

You can enter a stage-by-stage profile, or specify a top-stage pressure and a pressure drop for the rest of the column. For this example, use a condenser pressure of 16 psia, and a reboiler pressure of 20.2 psia. Aspen Plus interpolates the pressure of the intermediate stages.

8 In the **View** list, click and select **Pressure profile**.

9 In the first **Stage** field, type **1** and then press the **Tab** key.

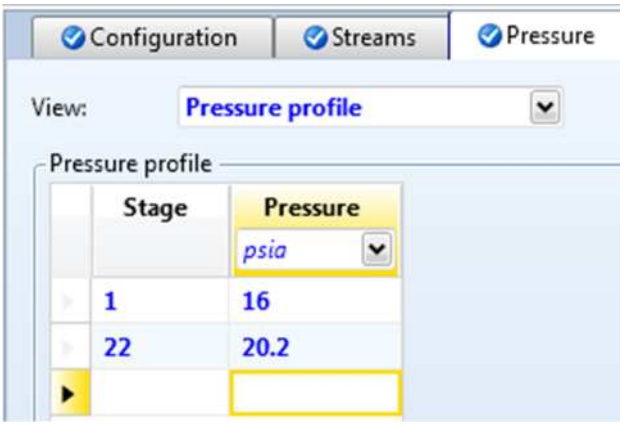
10 In the first **Pressure** field, type **16** and press **Tab**.

11 In the next **Stage** field, type **22** and press **Tab.**

12 In the next **Pressure** field, type **20.2** and press **Enter**.

13 Accept the default Pressure units (psia).

The completed **B1 (RadFrac) -Setup | Pressure** sheet looks like this:



14 Click .

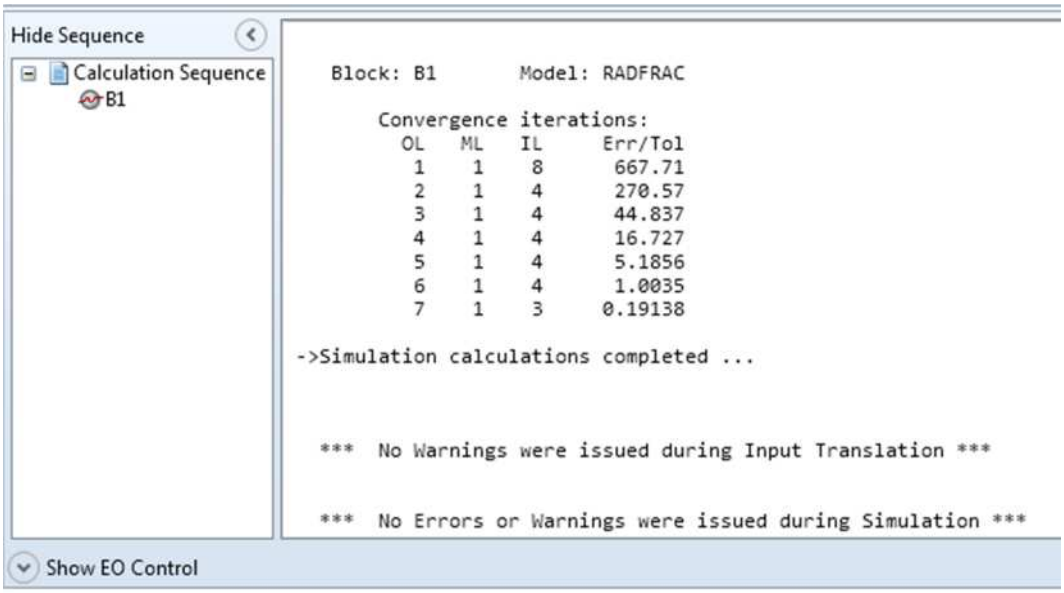
The **Required Input Complete** dialog box appears.

Note: You can enter additional specifications on optional input sheets, or go back to any of the required sheets and make changes. To see what optional input sheets are available, click **Cancel** on the **Required Input Complete** dialog box and navigate through the Navigation Pane to view all the folders. The **Reactions, Convergence, Flowsheeting Options,** and **Model Analysis Tools** folders are optional.

Running the Simulation

From the **Required Input Complete** dialog box, click **OK**.

The Control Panel appears and the simulation run begins:



Use the Control Panel to monitor and interact with the Aspen Plus simulation calculations. For more information on how to use the Control Panel, see the topic **Control Panel: about** in the online help index.

As Aspen Plus executes the simulation, status messages appear in the Control Panel. When the simulation is complete, the message *Results Available* appears on the status bar at the bottom of the main window.

The **Economic Analysis** dialog box appears. If you want to evaluate the capital and operating costs, make sure that you have installed and have a valid license for Aspen Process Economic Analyzer before clicking **Activate**.

Note: Click the tabs at the head of the active forms to navigate between different windows. For example, to view the Flowsheet, click the Main Flowsheet tab.

Examining Simulation Results

Now you can examine the results of your simulation.

1 Navigate to the process flowsheet in one of these ways:

- Click the **Main Flowsheet** tab, or
- Click the icon of **Flowsheet** on the Quick Access Toolbar, or
- Click **Flowsheet** in **Show** on the **View** tab of the ribbon

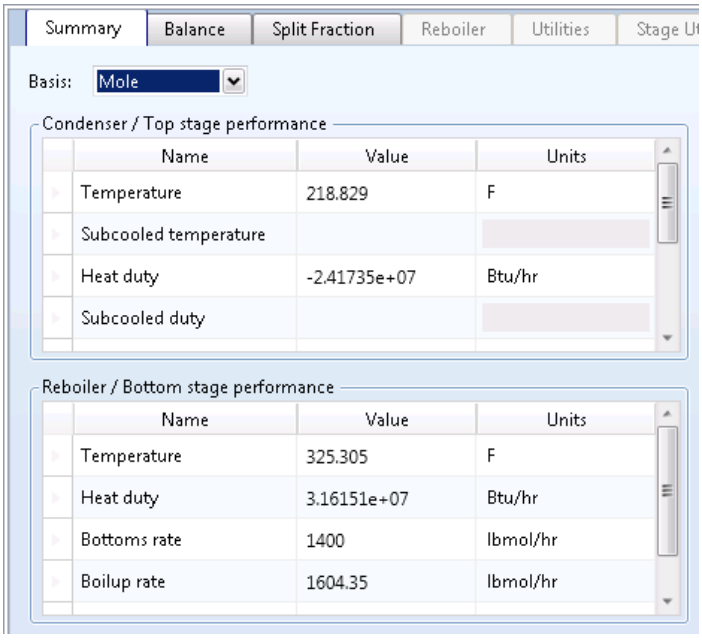
To Display the Results for Block B1

2 On the process flowsheet, select either the block name **B1** or the block itself, then right-click to display the shortcut menu.

Note: You may wish to alter the appearance of your flowsheet by using the **Zoom** tools on the **View** tab of the ribbon, for example**, Zoom to Fit**.

3 From the shortcut menu, select **Results**.

The **B1 (RadFrac) - Results | Summary** sheet appears:



For this run, block results are reported on three forms**: Results, Profiles,** and **Stream Results**. On the Navigation Pane, a check mark in a square appears next to each form to indicate that they contain results.

4 From the Navigation Pane, select **Blocks | B1 | Profiles** by clicking once on **Profiles**.

The **B1 (RadFrac) - Profiles | TPFQ** sheet appears, reporting temperature, pressure, heat duty, and flow profiles for the block:

TPFQ | Compositions | K-Values | Hydraulics | Reactions | Efficiencies | Propertie

View: All Basis: Mole

Stage	Temperature	Pressure	Heat duty	Liquid from (Mole)	Vapor from (Mole)
	F	psia	Btu/hr	lbmol/hr	lbmol/hr
1	218.829	16	-2.41735e+...	1800	0
2	219.689	16.2	0	1599.83	1800
3	220.59	16.4	0	1598.44	1799.83
4	221.585	16.6	0	1594.19	1798.44
5	222.835	16.8	0	1580.6	1794.19
6	225.037	17	0	1504.54	1780.6
7	235.917	17.2	0	2892	1704.54
8	236.868	17.4	0	2894.05	1892
9	237.883	17.6	0	2895.18	1894.05
10	239.003	17.8	0	2895.09	1895.18

5 Use the scrollbar(s) to view the displayed profiles.

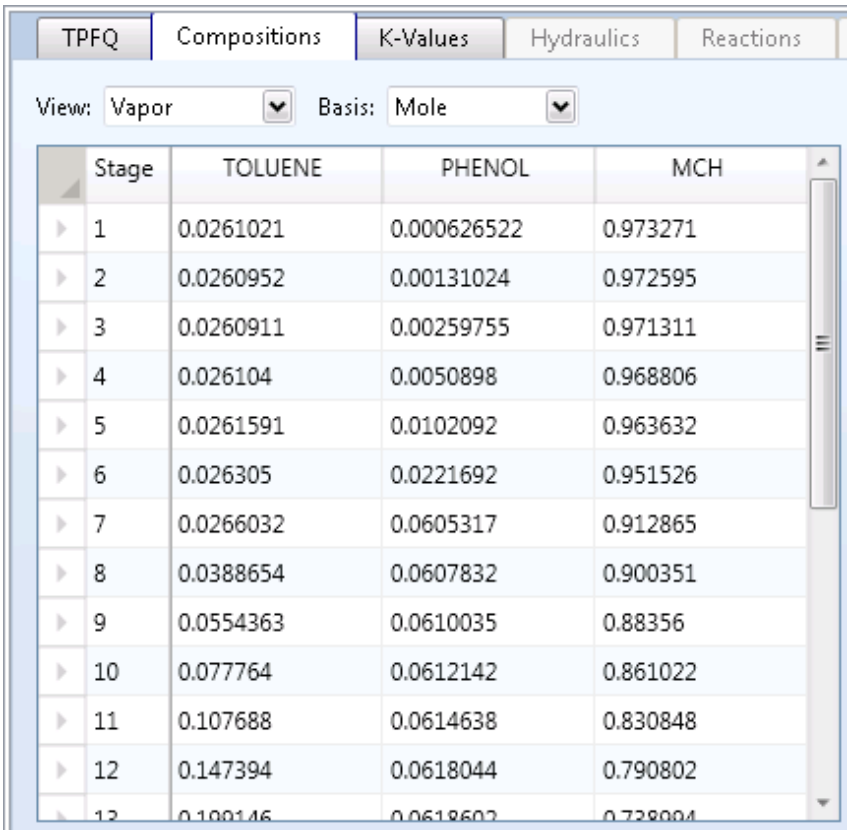
6 Click next to the **View** list and select **Stage flows**.

7 Use the **Basis** list to specify the type of units available for the displayed results.

8 Use the units box in each column to select the desired units for the display. Aspen Plus will perform the conversions automatically.

9 Use the Navigation Pane and the tabs on each form to view the rest of the results for Block B1. Click the **Compositions** tab.

10 Check the purity of the methylcyclohexane overhead product by examining the composition at the top of the column (stage 1).



Stage	TOLUENE	PHENOL	MCH
1	0.0261021	0.000626522	0.973271
2	0.0260952	0.00131024	0.972595
3	0.0260911	0.00259755	0.971311
4	0.026104	0.0050898	0.968806
5	0.0261591	0.0102092	0.963632
6	0.026305	0.0221692	0.951526
7	0.0266032	0.0605317	0.912865
8	0.0388654	0.0607832	0.900351
9	0.0554363	0.0610035	0.88356
10	0.077764	0.0612142	0.861022
11	0.107688	0.0614638	0.830848
12	0.147394	0.0618044	0.790802
13	0.199146	0.0618602	0.738994

This simulation predicts a little better than 97% purity for the MCH product with the given stream and block specifications.

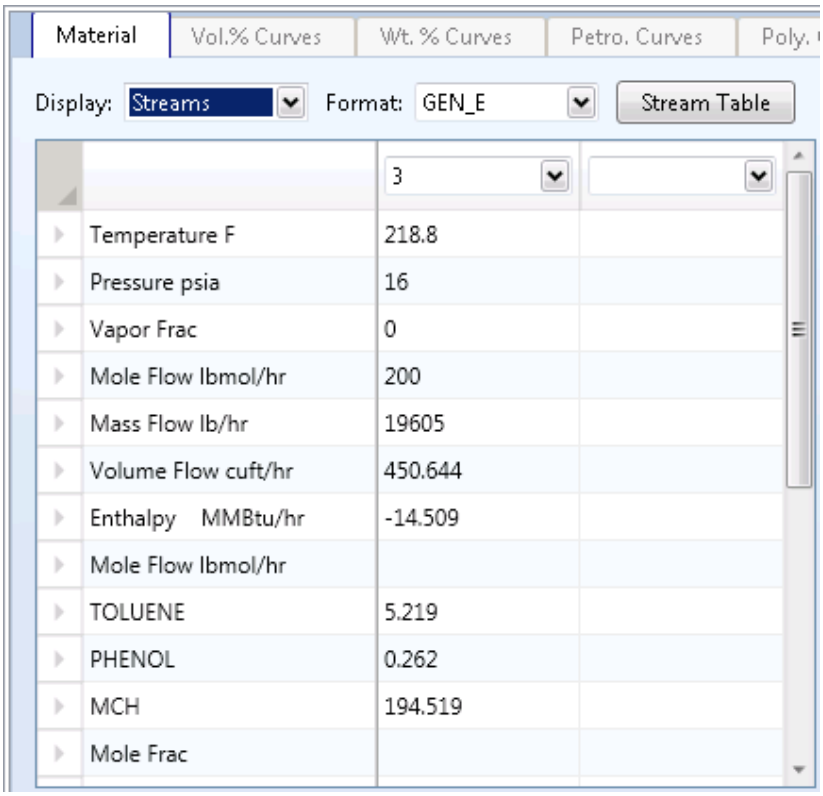
Examining Stream Results

Display calculated stream results by selecting a stream directly from the process flowsheet.

To Display the Results for Stream 3

1. Navigate to the process flowsheet.
2. Select Stream 3 and right-click to display the shortcut menu.
3. Select **Results.**

   The **3 (MATERIAL) - Results | Material** sheet appears, providing the results for Stream 3:



In addition to the thermodynamic state and flow results for the stream, mole fractions are also given (use the vertical scroll bar to view them) because you requested them by clicking the appropriate check box in the **Setup | Report Options | Stream** sheet.

To Display the Results for All Streams on the Same Sheet

1. On the **3 (MATERIAL) - Results | Material** sheet, click the box at the top of the first column of the data table (ignoring the field labels at the left) and select **1**.
2. Click the list box in the second column and select **2**.
3. Click the list box in the third column and select **3**.
4. Click the list box in the fourth column and select **4**.

   The results for all four streams are displayed. A quicker way to do this is to select **All streams** in the **Display** box.

Note: You can close some of the windows if you wish. Click the X at the right side of the window's tab to close that window.

Changing Input Specifications

In this section, review the effect of increasing the solvent flow rate on the purity and of the recovered methylcyclohexane.

To Increase the Phenol Solvent Stream Flow Rate

1 Navigate to the Flowsheet.

2 Select Stream 2, and right-click to display the shortcut menu.

3 Select **Input**.

The **2 (MATERIAL) | Mixed** sheet appears.

4 In the **Composition** field, change the flow rate for PHENOL from 1200 lbmol/hr to 1800 lbmol/hr by changing the entry in the **Value** field to **1800** and pressing **Enter** on the keyboard.

Since you have changed the input specifications, the symbols and appear in several places on the Navigation Pane. The (Run) command on the **Home** tab of the ribbon is now enabled.

Rerunning the Simulation with Changed Input

1 Click to continue.

The **Required Input Complete** dialog box appears indicating that your input is complete and asking if you want to run the simulation with the new specifications.

2 Click **OK** to run the simulation.

The column calculations are completed using the new phenol flow rate.

3 Display the new block and stream results by either selecting blocks and streams from the process flowsheet as before or navigating using the Navigation Pane.

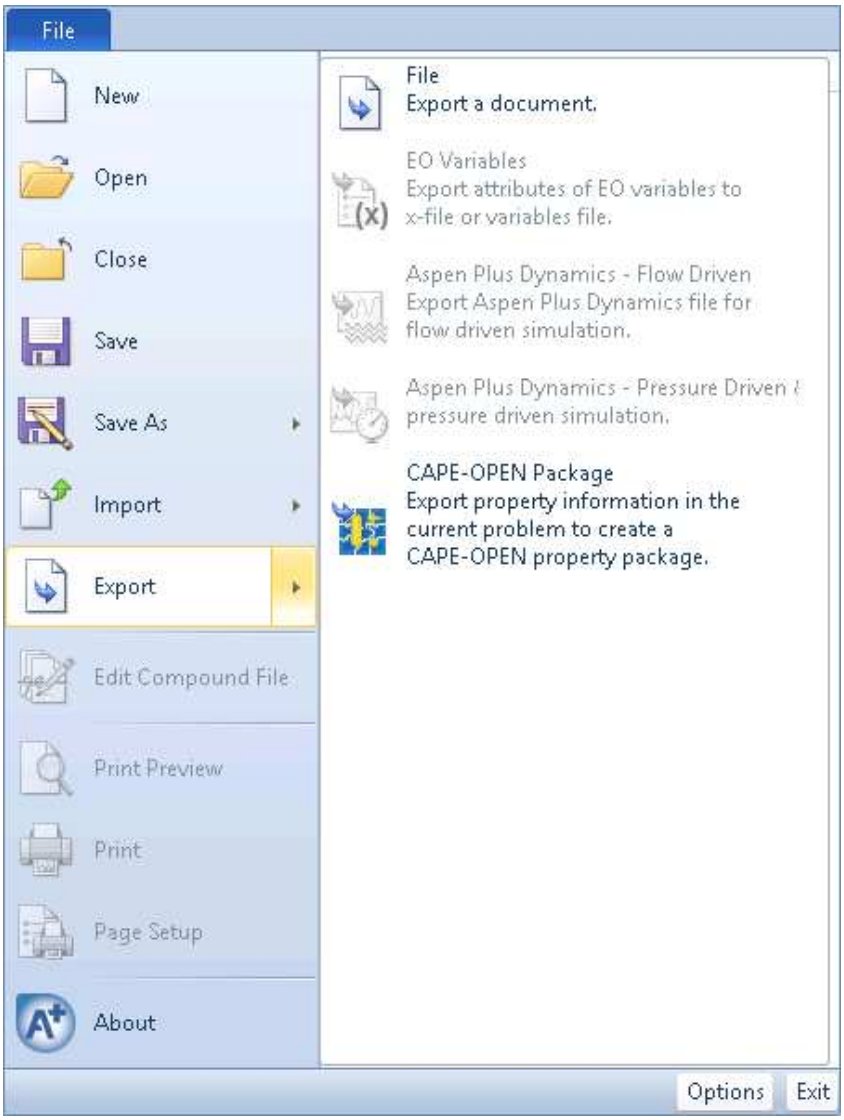
MCH purity with the increased phenol flow rate is now over 98%. To choose an optimal flow rate, it would be helpful to generate a plot of MCH purity versus phenol flow rate. This is the subject of Chapter 3 *Performing a Sensitivity Analysis*.

Creating Reports

To Generate a Report File

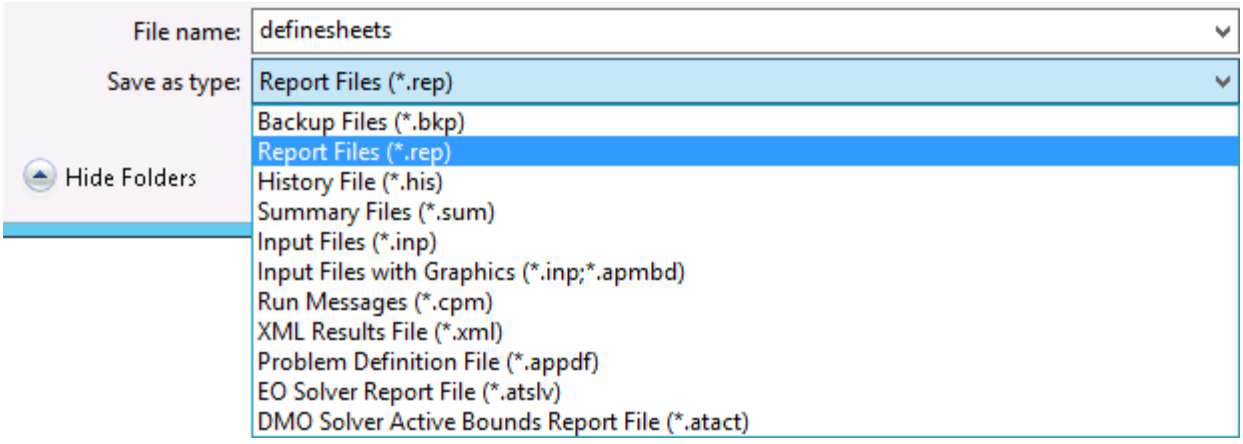
Aspen Plus allows you to generate a report file containing the simulation specifications and calculated results.

1 From the ribbon, select **File** and then move the cursor to **Export**.



A list appears on the right. Click **File**. The **Export** dialog box appears.

2 In the **Save as type** list, select **Report Files (*.rep)**.



3 In the **File name** field, type **MCH**.

4 Click **Save** to generate the report file, **MCH.rep**.

By default, **MCH.rep** is saved in your working directory (displayed in the **Save in** box). You can select another directory by navigating to it.

You can open **MCH.rep** with a text editor to read or print the file; it is not necessary to be running Aspen Plus at the same time. If you double-click on an Aspen Plus report file, it will be opened with a Windows text editor, most likely Notepad.

To View and Save Part of a Report

You can also examine the report before exiting Aspen Plus by clicking **Report** in **Summary** on the **Home** tab of the ribbon. The **Report** dialog box allows you to select which part of the report you want to display (for example, data from Stream 1 only). Aspen Plus will display the selected part of the report (or the whole report, if you select **Simulation**) using Notepad. From the **Notepad** window, you can then save the report fragment you are currently viewing by selecting **File | Save as**.

Saving Your File and Exiting Aspen Plus

1 From the ribbon, click **File**, and move the cursor to **Save As**.

   A list appears on the right. Click **Aspen Plus Document**. The **Save As** dialog box appears.

2 In the **File name** field, type **MCH**. Make sure the **Save as type** field reads **Aspen Plus Documents (*.apw)** and click **Save.**

   Aspen Plus saves the simulation in your working folder.

   Note: This folder is located in C:\Program Files\AspenTech\Working Folders\Aspen Plus <version> if C:\Program Files\AspenTech is the Root Directory selected when Aspen Plus was installed.

3 Select **File | Exit** to exit Aspen Plus.

Chapters 3 and 5 use **MCH.apw** as their starting point.

3 Performing a Sensitivity Analysis

One of the benefits of a simulation is that you can study the sensitivity of process performance to changes in operating variables. With Aspen Plus, you can allow inputs to vary, and can tabulate the effect on a set of results of your choice. This procedure is called a sensitivity analysis.

In this chapter, you will perform a sensitivity analysis using either the methylcyclohexane (MCH) recovery simulation you created in Chapter 2 or the MCH simulation that was placed in the **Examples** folder when you installed Aspen Plus.

Allow about 20 minutes for this simulation.

Starting Aspen Plus

1. From your desktop, select **Start** and then select **Programs.**
2. Select **AspenTech | Process Modeling <version> | Aspen Plus | Aspen Plus <version>**.

   The **Start Using Aspen Plus** window appears in the main window.

Opening an Existing Simulation

You can open a saved simulation file from the list presented at startup, or by navigating to a folder containing the saved file. For this session, either open your saved **MCH.apw** from Chapter 2, or use **MCH.bkp** in the **Examples\GSG_Process** folder.

If Your Saved File MCH.apw is Displayed

To open an existing simulation:

1 On the **Start Using Aspen Plus** window, find **Recent Models**.

2 In the list, select **MCH.apw** and click **OK**.

If Your Saved File MCH.apw is not Displayed

1 Click **File** on the ribbon and select **Open**.

The **Open** dialog box appears.

2 Navigate to the directory containing your saved **MCH.apw** or navigate to the **Examples\GSG_Process** folder containing **MCH.bkp**.

Note: The **Examples** folder is located in: C:\Program Files\AspenTech\Aspen Plus <version>\Favorites\Examples, if C:\Program Files\AspenTech is the Root Directory selected when Aspen Plus was installed.

3 Select either **MCH.apw** or **MCH.bkp** and click **Open**.

The **Flowsheet** window of the MCH column simulation appears.

Saving a Simulation under a New Name

Before creating a new simulation from MCH.apw or MCH.bkp, create a file with a new name, **MCHSENS.apw**. Now you can modify this new file. The original is safe.

1 From the ribbon, click **File** and then move the cursor to **Save As.**

2 In the **Save As** list which appears on the right side, select **Aspen Plus Document**.

The **Save As** dialog box appears.

3 Choose the directory where you want to save the simulation from the **Look in** list.

4 In the **File name** field, enter **MCHSENS**.

5 Click **Save**.

Defining the Sensitivity Analysis

In Chapter 2, you simulated MCH recovery using two values for the phenol solvent flow rate. In the following sensitivity analysis, tabulate methylcyclohexane (MCH) distillate product purity (mole fraction), as well as condenser duty and reboiler duty, for several different flow rates of phenol.

To do this, you must make sure that you are in the **Simulation** environment by checking that the **Simulation** bar is highlighted on the Navigation Pane.

Entering Sensitivity Specifications

To Create a New Sensitivity Block

1. Select **Model Analysis Tools | Sensitivity**.

   The **Sensitivity** object manager appears.

   You can use this sheet to:

   - Create new sensitivity blocks.
   - Edit existing sensitivity blocks.
   - View status of sensitivity blocks.
2. Click **New**.

   The **Create New ID** dialog box appears.
3. Click **OK** to accept the default ID **S-1**.

   The **S-1 | Vary** sheet appears.

This sensitivity analysis will generate a data table. The first column will contain a user-specified range of input values for the phenol flow rate. Three other columns will contain calculated results for MCH distillate product purity, the condenser duty, and the reboiler duty.

In the **Vary** sheet, specify the range and increments for the manipulated variable (phenol flow rate). In the **Define** sheet, define names for each of the calculated variables (product purity, condenser duty, reboiler duty). In the **Tabulate** sheet, set up the format you want for the data table.

Start with the definition of the MCH distillate product purity variable.

To Specify the Manipulated Variable

Define the phenol flow rate (Stream 2) to vary from 1200 lbmol/hr to 2000 lbmol/hr in increments of 100 lbmol/hr.

1. In the **Edit selected variable** section, click  beside the **Variable** field, select **<New>.** The value of this field then changes to **1**.

2 In the **Type** field, select **Stream-Var**.

3 In the **Stream** field, select **2**. The **Substream** and **Variable** fields appears. **MIXED** has been selected as the Substream. You need to fill in the Variable field.

While you could click and search for Mole Flow, the list of Stream Variables is not very long, so you may find it easier to pick from a list. Both methods of identifying and selecting variables are acceptable.

4 In the **Variable** field, click and select **MOLE-FLOW**.

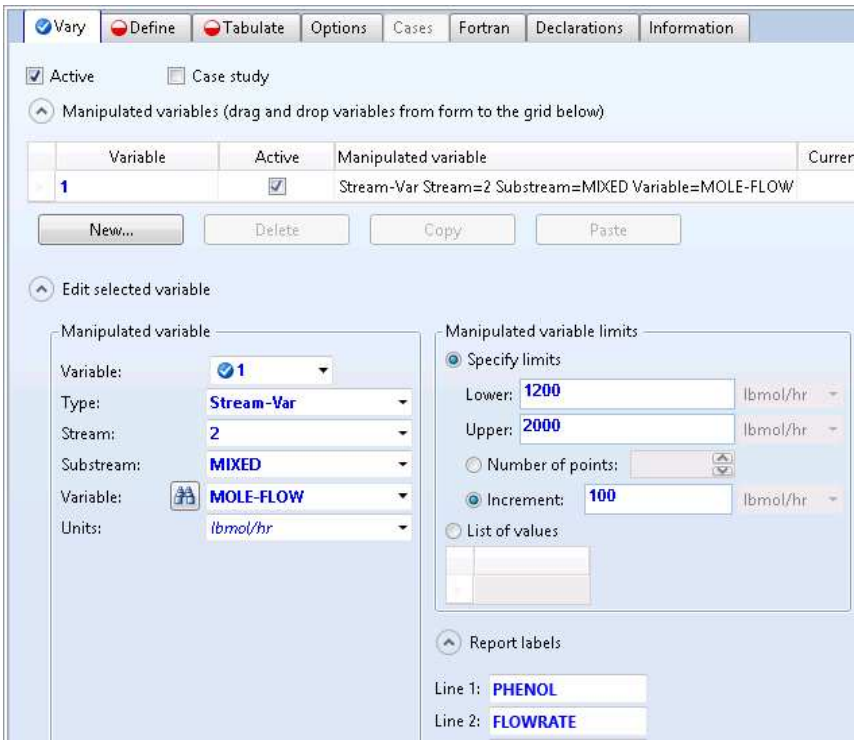
5 In the **Manipulated variable limits** area, select **Specify limits** and **Increment** and enter the following values:

Field	Value
Lower	1200
Upper	2000
Increment	100

6 Click to open the **Report labels** area. Here you have the option of entering up to four lines to be used as a column header in the Sensitivity table. Enter the following report labels:

Line	Value
Line 1	PHENOL
Line 2	FLOWRATE

You have completely specified the phenol flow rate as a manipulated variable for this sensitivity analysis:



Next, define the variables.

To Define XMCH as Distillate Product Purity

1 Click or click the **Define** tab. On the **Define** sheet, click **New**.

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

2 Type **XMCH** and click **OK**.

The variable XMCH appears in the **Edit selected variable** section. Define XMCH to be the mole fraction of MCH in Stream 3 as follows.

3 In the **Category** area, select **Streams**.

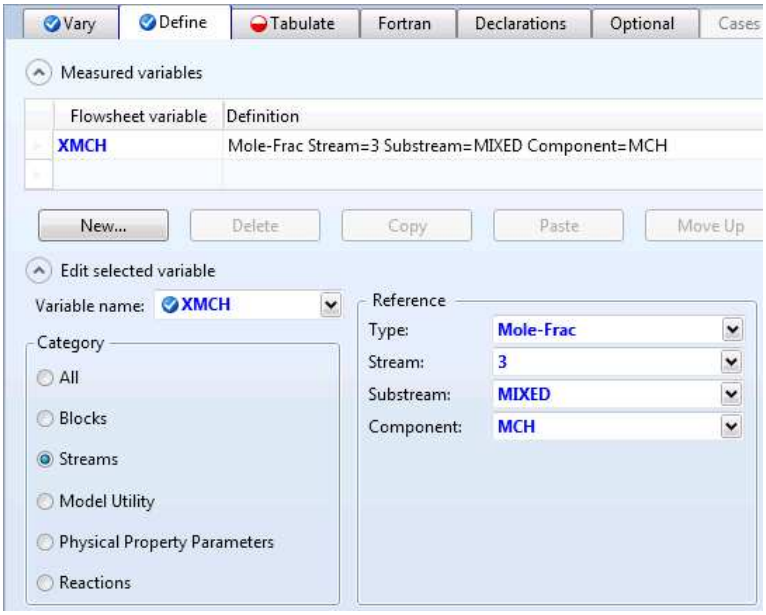
4 In the **Reference** area, click the **Type** field and select **Mole-Frac**.

5 In the **Stream** field, select **3**.

In this simulation, you do not need to modify the default value of MIXED in the Substream field.

6 In the **Component** field, select **MCH**.

You have defined XMCH to be the mole fraction of MCH in Stream 3. The blue checkmarks indicate that the variable specification is complete.



Next, define the condenser duty and reboiler duty variables.

To Define QCOND as the Condenser Duty and QREB as Reboiler Duty

1 Click **New** again.

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

2 Type **QCOND** and click **OK**.

3 In the **Variable** list, select QCOND. Now define QCOND to be the condenser duty for the RadFrac Block B1.

4 In the **Category** area, select **Blocks**.

5 In the **Type** field, select **Block-Var**.

6 In the **Block** field, select **B1**.

7 In the **Variable** field, click  to show the list of variables.

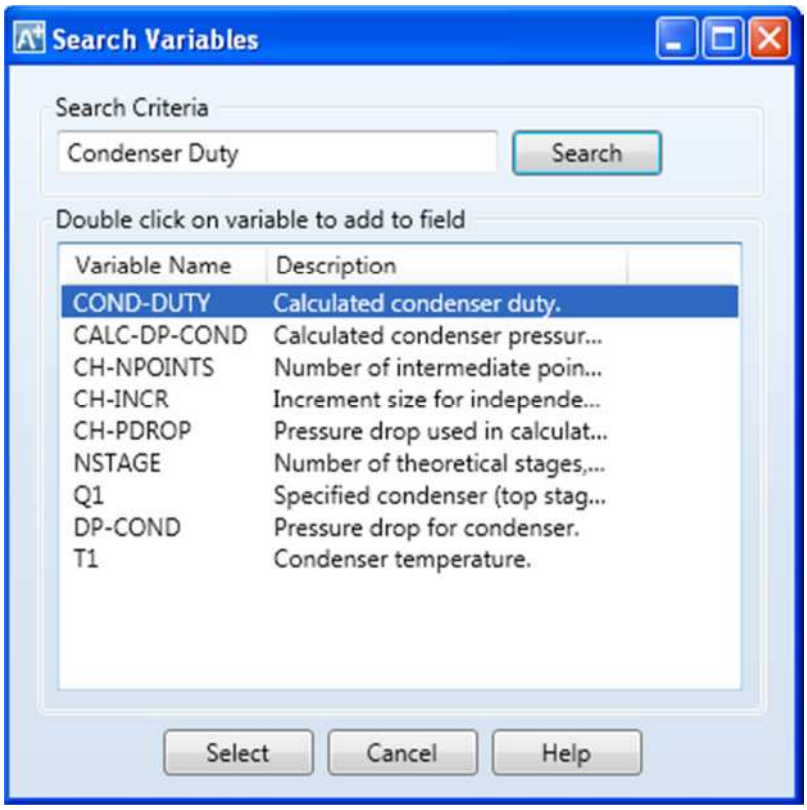
Judging by the size of the scroll bar, the list of variables is quite long. For complex unit operation models like RadFrac, it can be difficult to find the intended variable. Aspen Plus offers a search capability to help you find the correct variable.

8 Click the icon  next to the **Variable** list.

The **Search Variables** dialog box appears. You can search on any string that you think might help to reduce the number of variables.

9 In the **Search Criteria** area, enter **Condenser Duty**.

Aspen Plus searches for variables that contain the words Condenser and Duty in the variable name or variable description. The search is not case sensitive. Aspen Plus identifies the following variables:



10 Double-click **COND-DUTY** to select it as the simulation variable linked to the variable you have named QCOND.

Aspen Plus automatically fills in the **Sentence** field and the **Units** field, based on your choice of variable. Aspen Plus also shows the units of measure for the accessed variable (Btu/hr).

Note: The units of measure for accessed variables depend on the units of measurement of the object that contains the defined variables. Since this Sensitivity blocks uses ENG units, heat duties have the units of Btu/hr. If you were to toggle the units to SI, the heat duties would be accessed in Watts.

Now define the next variable, QREB.

11 In the **Variable** field, click and select **<New>**.

Note: You can also right-click on the **Variable** field and from the shortcut menu, select **Create**.

The **New Item** dialog box appears.

12 Type **QREB** and click **OK**.

Define QREB to be the reboiler duty for Block B1.

13 In the **Category** area, select **Blocks**.

14 In the **Type** field, select **Block-Var**.

15 In the **Block** field, select **B1**.

16 Click next to the **Variable** list, and search for **Reboiler Duty**.

17 Double click **REB-DUTY** to select it as the simulation variable linked to the variable you have named QREB.

Aspen Plus fills in the **Variable**, **Sentence** and **Units** of measure for QREB.

You have now defined QCOND and QREB to be the condenser duty and reboiler duty for block B1.

The **S-1 | Define** sheet reappears with the three defined calculated variables, XMCH, QCOND, and QREB listed.

Next, specify the format for the table that Aspen Plus will produce when you run the analysis.

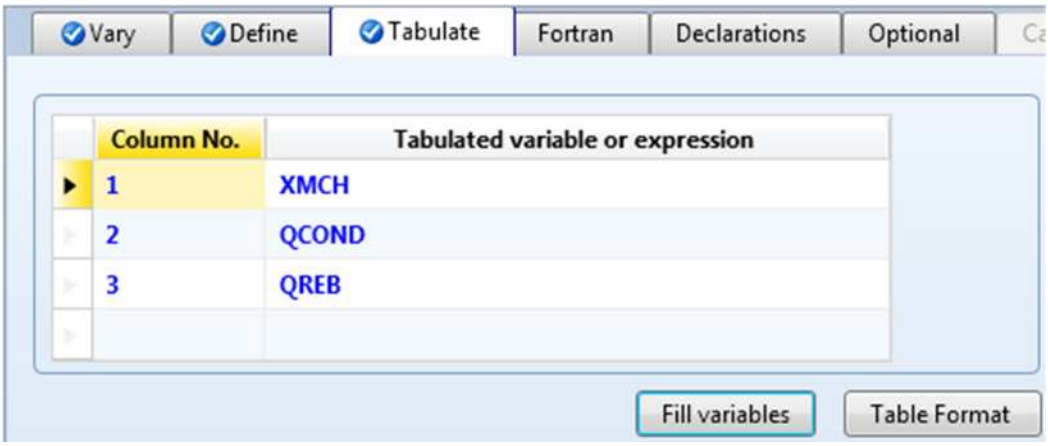
To Format the Tabular Results

1 Click or click the **Tabulate** tab.

The **S-1 | Tabulate** sheet appears. You must identify the variables that you want to appear in the Sensitivity table.

2 Click **Fill variables** to have Aspen Plus tabulate all of the defined variables automatically.

The completed sheet looks like this:



Note: You could have filled out the same information manually. You can also tabulate mathematical expressions written using Fortran notation.

3 Click **Table Format**.

The **Table Format** dialog box appears. Enter column labels for columns 1, 2, and 3, whose data contents were defined above.

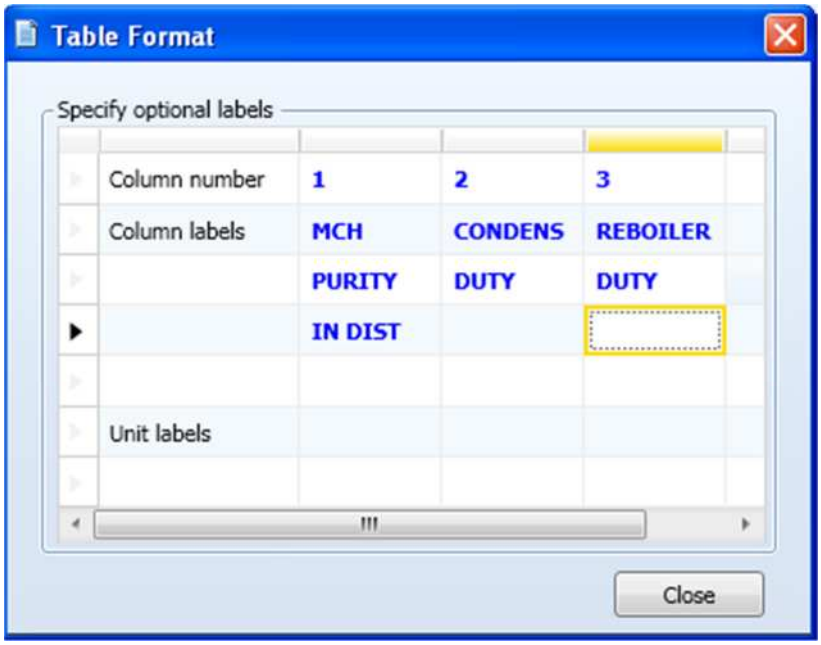
Labels are split into 4 lines for the report file. Each line can contain up to 8 characters.

4 In column 1 type **MCH PURITY IN DIST** using 3 lines.

5 In column 2 type **CONDENS DUTY** using 2 lines.

6 In column 3 type **REBOILER DUTY** using 2 lines.

The completed dialog box looks like this:



7 Click **Close**.

The **S-1** form is complete and you are ready to run the sensitivity analysis.

Running the Sensitivity Analysis

Run the simulation in any of the following ways:

- From the **Home** tab of the ribbon, in **Run**, click .
- Press **F5**.

Now you can display and plot the results.

Displaying Sensitivity Analysis Results

The Sensitivity Analysis Results consist of a table of the values you requested on the **Tabulate** sheet, shown as a function of the manipulated variable defined on the **Vary** sheet.

1 From the Navigation Pane, click **Model Analysis Tools | Sensitivity | S-1 | Results**.

The **S-1 - Results | Summary** sheet appears:

Summary | Define Variable | Status

Row/Case	Status	VARY 1 PHENOL FLOWRATE LBMOL/HR	MCH PURITY IN DIST	CONDENS DUTY BTU/HR	REBOILER DUTY BTU/HR
1	OK	1200	0.972595	-2.41735E+07	3.16151E+07
2	OK	1300	0.975346	-2.41703E+07	3.2358E+07
3	OK	1400	0.977698	-2.41676E+07	3.31097E+07
4	OK	1500	0.979708	-2.41653E+07	3.38685E+07
5	OK	1600	0.981433	-2.41634E+07	3.46336E+07
6	OK	1700	0.982924	-2.41617E+07	3.54042E+07
7	OK	1800	0.984217	-2.41603E+07	3.61795E+07
8	OK	1900	0.985346	-2.4159E+07	3.6959E+07
9	OK	2000	0.986336	-2.4158E+07	3.77421E+07

Note: The above results were obtained using the Aspen Plus document file, mch.apw. If you used the Aspen Plus backup file, mch.bkp, from the **Examples** folder, your results may be slightly different (in the 3rd significant digit or beyond). These differences occur because the starting points for the iterative calculations are different. When you use an .apw file, Aspen Plus starts calculating from the previous results. When you use a .bkp file, Aspen Plus reinitializes before starting calculations.

Plotting Sensitivity Results

Make a plot of MCH purity vs. phenol flow rate.

To Generate a Plot of MCH Distillate Purity Versus Phenol Flow Rate

1 From the **Home** tab of the ribbon, in **Plot**, click **Results Curve**. The **Results Curve** dialog box appears.

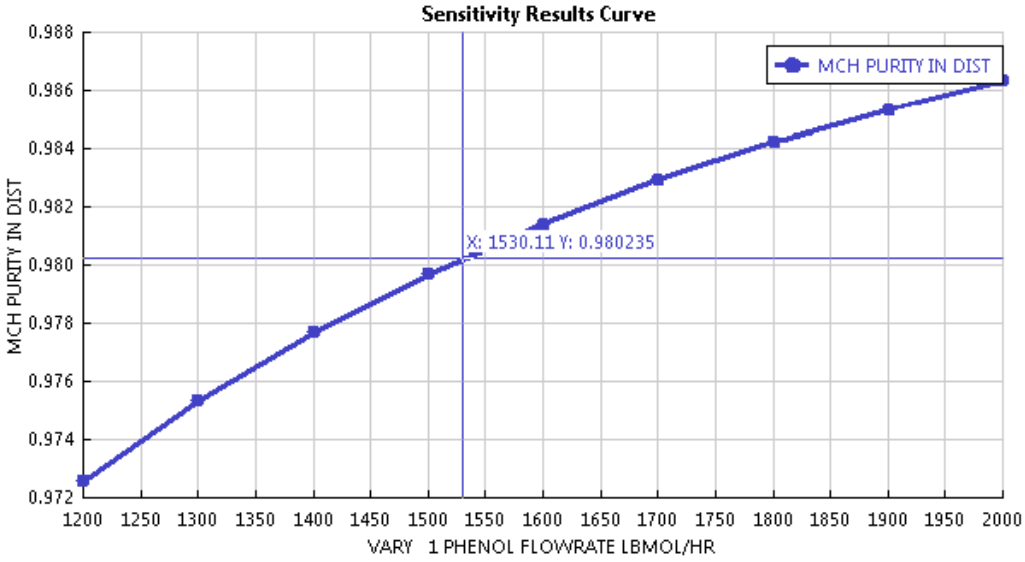
2 In the **X Axis** field, verify that **VARY 1 PHENOL FLOWRATE** is selected.

3 In the field **Select curve(s) to plot**, make sure that only the check box in front of **MCH PURITY IN DIST** is selected.

4 Click **OK**.

A new window appears containing the plot you specified.

5 In the **Format** tab on the ribbon, in the Display group, click the checkbox for Tracker. This turns on a crosshair that moves with the mouse pointer, but remaining on the variable line. It shows the X and Y value at the currently selected point (interpolating between the calculated values).



You can modify other aspects of the plot from this ribbon tab.

Saving Your File and Exiting Aspen Plus

1 From the ribbon, click **File** and select **Exit**.

2 Click **OK** to save to simulation and exit.

Chapter 4 uses **MCHSENS.apw** as its starting point.

4 Meeting Process Design Specifications

In Chapter 3, you used Aspen Plus to tabulate the sensitivity of MCH distillate purity and column duties to changes in phenol solvent flow rate. You can also use Aspen Plus to meet a specific process design target (or design specification) by manipulating any simulation input variable.

In this chapter, you will use Aspen Plus to meet a process design specification using either the methylcyclohexane (MCH) recovery simulation you created in Chapter 2 or the MCH simulation that was placed in the **Examples** folder when you installed Aspen Plus.

Allow about 20 minutes for this simulation.

Starting Aspen Plus

1 From your desktop, select **Start** and then select **Programs**.

2 Select **AspenTech | Process Modeling <version> | Aspen Plus | Aspen Plus <version>**.

The **Start Using Aspen Plus** window appears in the main window.

Opening an Existing Simulation

You can open a saved simulation file from the list presented at startup, or by navigating to a folder containing the saved file. For this session, either open your saved **MCHSENS.apw** from Chapter 3, or use **MCHSENS.bkp** in the **Examples** folder.

If Your Saved MCHSENS.apw is Displayed

To open an existing simulation:

1 On the **Start Using Aspen Plus** window, find **Recent Models**.

2 In the list, select **MCHSENS.apw** and click **OK**.

If Your Saved File MCHSENS.apw is Not Displayed

1 Click **File** on the ribbon and select **Open**.

The **Open** dialog box appears.

2 Navigate to the directory containing your saved **MCHSENS.apw** or navigate to the **Examples\GSG_Process** folder containing **MCHSENS.bkp**.

Note: The **Examples** folder is located in: C:\Program Files\AspenTech\Aspen Plus <version>\Favorites\Examples if C:\Program Files\AspenTech is the Root Directory selected when Aspen Plus was installed.

3 Select either **MCHSENS.apw** or **MCHSENS.bkp** and click **Open**.

Saving a Simulation Under a New Name

Before creating a new simulation from **MCHSENS.apw** or **MCHSENS.bkp**, create a file with a new name, **MCHSPEC.apw**. Now you can modify this new file. The original is safe.

1 From the ribbon, click **File** and then move the cursor to **Save As**. Click **Aspen Plus Document**.

2 In the **Save As** dialog box, choose the directory where you want to save the simulation.

3 In the **File name** field, enter **MCHSPEC**.

4 Click **Save**.

Defining the Design Specification

In Chapter 2, you simulated MCH recovery using two values for the phenol solvent flow rate. In the sensitivity analysis in Chapter 3, you tabulated MCH distillate product purity, and condenser and reboiler duties, as a function of phenol solvent flow rate.

Now use Aspen Plus to determine the exact phenol solvent feed rate required to maintain an MCH distillate purity of 98%.

To Enter Design Specifications

1 Select **Flowsheeting Options | Design Spec** in the Navigation Pane.

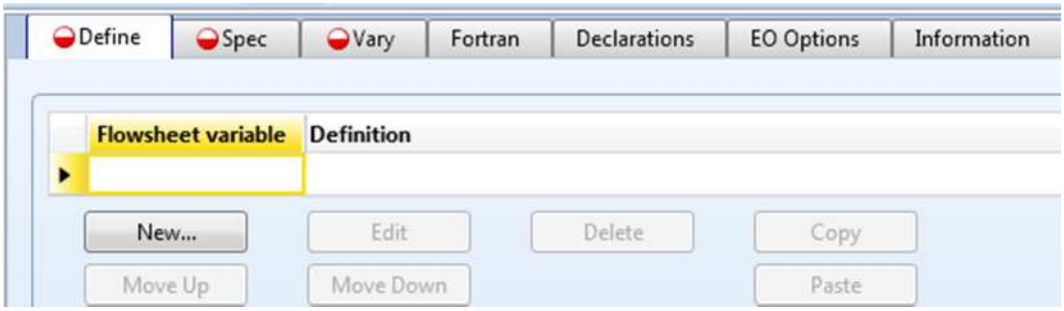
The **Design Spec** object manager appears.

2 Click **New**.

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

3 Click **OK** to accept the default ID **DS-1**.

The **DS-1 | Define** sheet appears:



In the **Define** sheet, define XMCH to be the MCH purity. In the **Spec** sheet, enter the specification as a mathematical expression containing numbers and defined variables, and also enter a target value for this expression and a tolerance. In the **Vary** sheet, specify an input variable to be manipulated and a range in which Aspen Plus will search in order to obtain the target value given on the **Spec** sheet.

Start with the definition of XMCH as the mole fraction of MCH in Stream 3.

To Define XMCH in DS-1

XMCH is already defined in Sensitivity S-1. Rather than recreate it in DS-1, you will copy it from the Sensitivity.

1 In the Navigation Pane, expand **Model Analysis Tools**, **Sensitivity**, and **S-1**.

2 Right-click **Input** under **S-1** to open the shortcut menu. Select **Open in new tab**. The **S-1 - Input | Vary** sheet of Sensitivity S-1 appears on a different tab beside the **DS-1** tab in the workspace area.

3 Click the **Define** tab.

S-1 - Input | Define sheet appears.

4 Select **XMCH**, and click **Copy**.

5 Click the tab header **DS-1**. The **Define** sheet for Design-Spec DS-1 appears.

6 Click **Paste**. A new variable is copied to Design-Spec DS-1. Type **XMCH** in the **Flowsheet variable** column as the name for the new variable.

The **DS-1 | Define** sheet has the defined variable, XMCH, listed.

Next, set up the following design specification: the percentage of recovered MCH must be 98.0 within a tolerance 0.01.

To Set Up the Design Specification

1 Click or click **Spec**.

The **DS-1 | Spec** sheet appears.

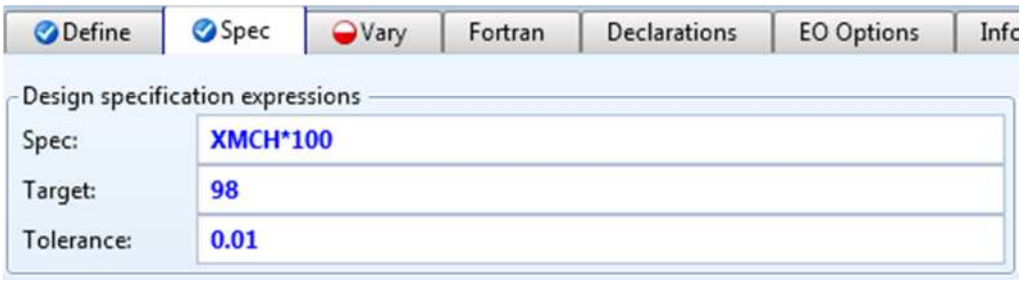
2 In the **Spec** field, type **XMCH*100**.

The multiplicative factor of 100 converts the sampled mole fraction to a mole percentage.

3 In the **Target** field, enter **98**.

4 In the **Tolerance** field, enter **0.01** to specify an acceptable deviation from the target percentage.

The completed sheet looks like this:



Next, specify the phenol flow rate (Stream 2) as the variable you want Aspen Plus to manipulate in order to achieve the above design specification. Give a range of 1200 to 2000 within which Aspen Plus will search.

To Specify the Manipulated Variable

1 Click or click **Vary**.

The **DS-1 | Vary** sheet appears.

2 In the **Manipulated variable** area, click the **Type** field and select **Stream-Var**.

3 In the **Stream** field, select **2**.

4 In the **Substream** field, accept the default, **MIXED**.

5 In the **Variable** field, select **MOLE-FLOW**.

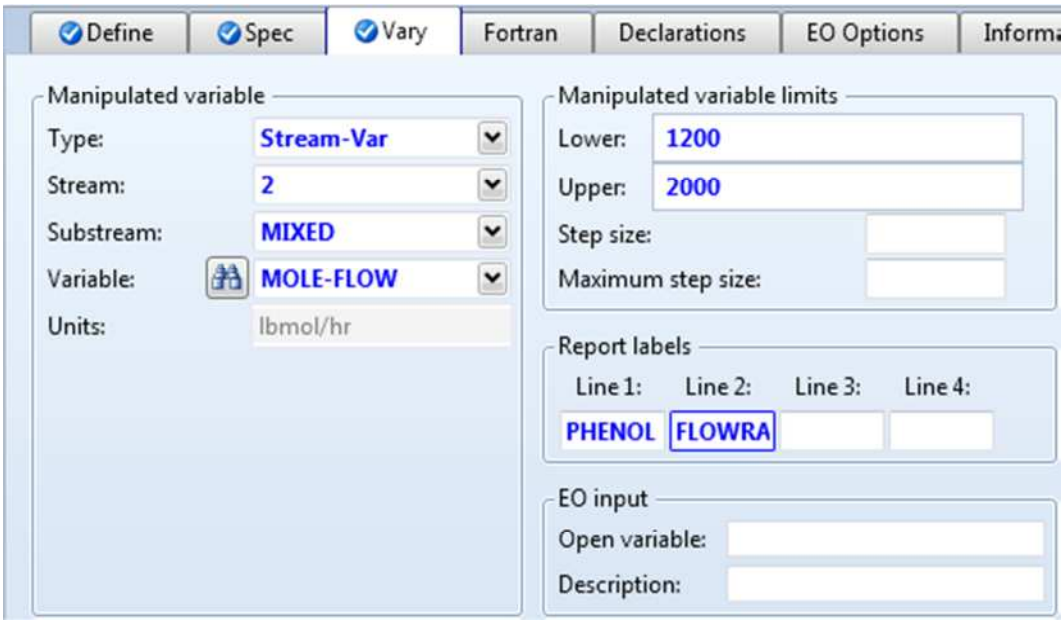
6 In the **Manipulated variable limits** area, click the **Lower** field and type **1200**.

7 In the **Upper** field type **2000**.

8 In the **Report labels** area, click the **Line 1** field and type **PHENOL**.

9 In the **Line 2** field, type **FLOWRATE**.

The completed sheet looks like this:



The **DS-1** form is complete. However, Sensitivity S-1 still exists. Before running the design specification analysis, you must hide Sensitivity S-1.

To Hide Sensitivity S-1

1 Select **Model Analysis Tools | Sensitivity** from the Navigation Pane. The **Sensitivity** Object Manager appears.

2 Select row **S-1**, and click **Hide**. Click **OK** to confirm. Sensitivity S-1 disappears from the object manager. Hidden objects no longer have an active role in the current simulation.

Note: Many of the object managers in Aspen Plus have the capability to hide individual objects. If an object manager has hidden objects, **Reveal** will be active. Click **Reveal** to reveal one or more hidden objects.

You are ready to run the design specification analysis and examine the results.

Running the Design Specification Analysis

Run the analysis in any of the following ways:

- From the ribbon, on the **Home** tab, click in the **Run** group.
- Press **F5**.

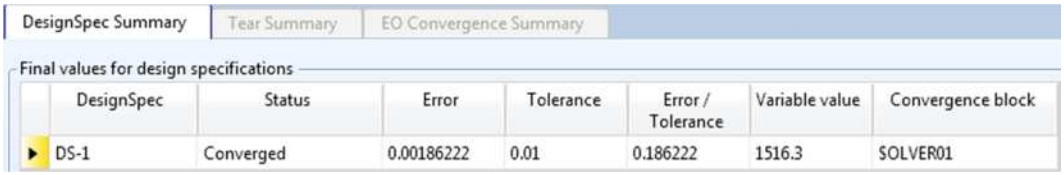
Then examine the results.

Examining Design Specification Results

Determine how well your design specification has been satisfied by examining the **Results Summary - Convergence | DesignSpec Summary** sheet.

1 From the Navigation Pane tree, click **Results Summary | Convergence**.

The **Results Summary - Convergence | DesignSpec Summary** sheet appears:



DesignSpec	Status	Error	Tolerance	Error / Tolerance	Variable value	Convergence block
DS-1	Converged	0.00186222	0.01	0.186222	1516.3	SOLVER01

The results show that that the calculation converged successfully and that the necessary value of the phenol flow rate is approximately 1515.0. The units, lbmol/hr, are not shown.

Note: The above results were obtained by using the Aspen Plus document file, **MCH.apw**. If you used the Aspen Plus backup file, **MCH.bkp**, from the **Examples** folder, your results may be slightly different (in the 3rd significant digit and beyond). These differences occur because the starting point for the calculations are different. When you use a document (.apw) file, Aspen Plus starts calculating from the previous results. When you use a backup (.bkp) file, Aspen Plus reinitializes before starting calculations.

Exiting Aspen Plus

1 From the ribbon, click **File** and select **Exit**.

The **Aspen Plus** dialog box appears.

2 Click **Yes** to save the simulation.

5 Annotating Process Flowsheets

In the Simulation environment, you can modify your process flowsheet to prepare customized drawings for reports by:

- Displaying global data for streams and blocks
- Displaying stream results tables
- Adding text and graphics
- Adding a molecular structure symbol

In this chapter, you will annotate the process flowsheet you used in the MCH simulation. You can use the file created in Chapter 2 or the simulation that was saved in the **Examples** folder when you installed Aspen Plus.

Allow about 20 minutes for this example.

Starting Aspen Plus

1 From your desktop, select **Start** and then select **Programs**.

2 Select **AspenTech | Process Modeling <version> | Aspen Plus | Aspen Plus <version>**.

The **Start Using Aspen Plus** window appears in the main window.

Opening an Existing Simulation

You can open a saved simulation file from the list presented at startup, or by navigating to a folder containing the saved file. For this session, either open your saved **MCH.apw** from Chapter 2, or use **MCH.bkp** in the **Examples** folder.

If Your Saved File MCH.apw is Displayed

To open an existing simulation:

1 On the **Start Using Aspen Plus** window, find **Recent Models**.

2 In the list, select **MCH.apw** and click **OK**.

If Your Saved File MCH.apw is not Displayed

1 Click **File** on the ribbon and select **Open**.

The **Open** dialog box appears.

2 Navigate to the directory containing your saved **MCH.apw** or navigate to the **Examples\GSG_Process** folder containing **MCH.bkp**.

Note: The **Examples** folder is located in: C:\Program Files\AspenTech\Aspen Plus <version>\Favorites\Examples if C:\Program Files\AspenTech is the Root Directory selected when Aspen Plus was installed.

3 Select either **MCH.apw** or **MCH.bkp** and click **Open**.

The Process Flowsheet

The process flowsheet is used to create a graphical representation of your process for a report or for display purposes. Use the process flowsheet to do the following:

- Display stream data.
- Display a results table.
- Add a title.

To view the Flowsheet:

- Click **Flowsheet** from the Quick Access Toolbar above the ribbon.
- Click the **Main Flowsheet** tab in the workspace to display the process flowsheet.
- Click **Flowsheet** in **Show** on the **View** tab of the ribbon

Note: On the ribbon, the **Flowsheet** tab hides when you navigate away from the Flowsheet window in the workspace area.

Displaying Stream Data

To Display Temperature and Pressure

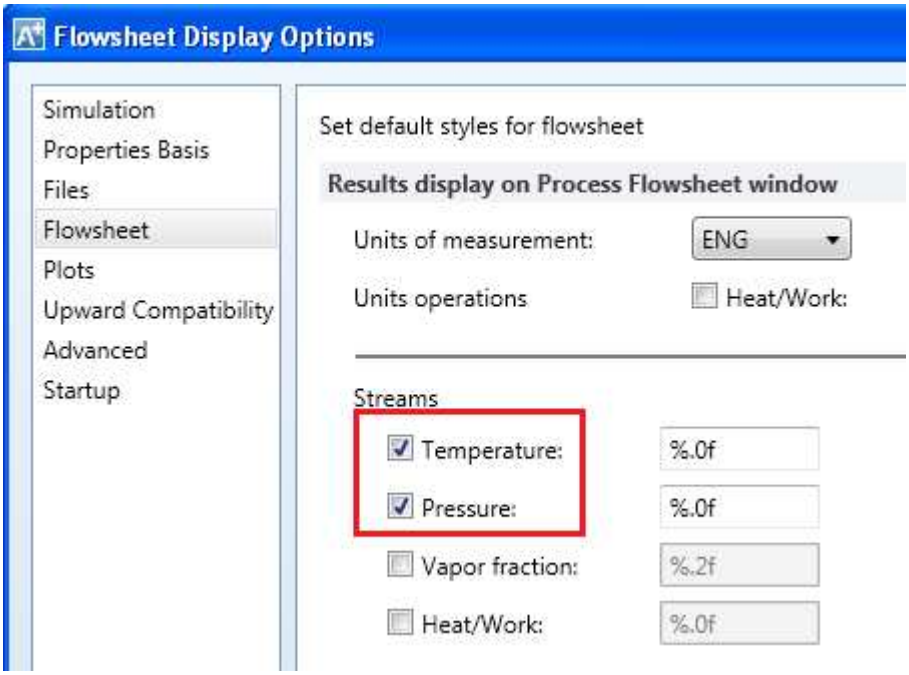
1 On the **Flowsheet | Modify** tab of the ribbon, click **Display Options**, and ensure that **Global Data** has a checkmark next to it.

Note: The tabs for **Flowsheet** only appear when the Flowsheet is active.

2 Click **File** on the ribbon, then click **Options**. The **Simulation Run Options** dialog box appears.

3 Click **Flowsheet** on the pane on the left to view Flowsheet Display Options.

4 Under **Results display on Process Flowsheet window**, select the **Temperature** and **Pressure** check boxes for **Streams**.

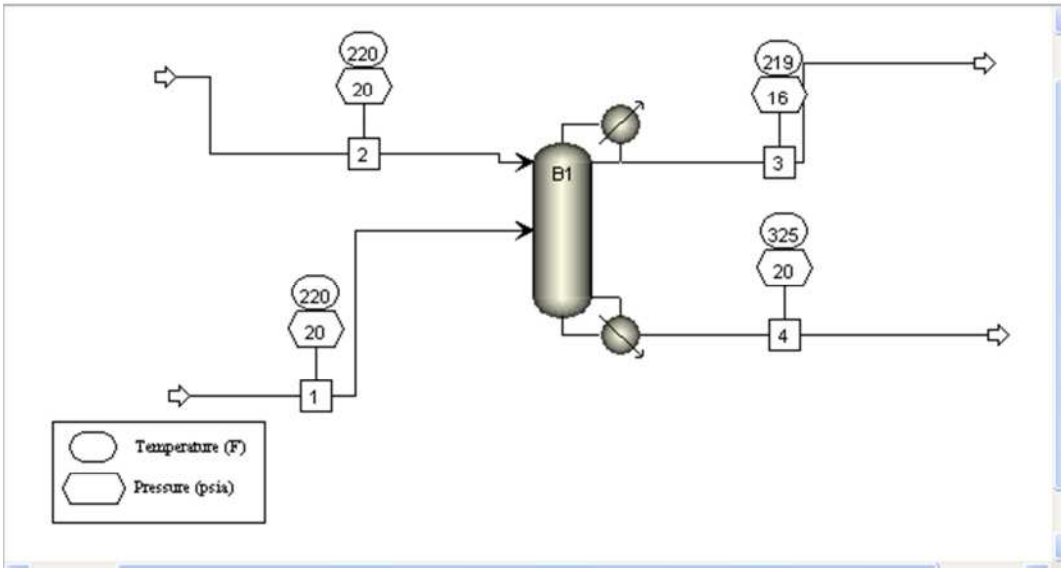


5 Click **Apply** and then **OK**.

The temperature and pressure calculated by Aspen Plus during the MCH simulation run are shown on each stream. Aspen Plus also displays a legend box in the lower left corner of the screen. The legend box shows the symbols and units for the global data. Move and resize the legend in the same way that you move and resize blocks.

Note: If you do not see the legend box, select **View | Zoom | Zoom to Fit** from the ribbon or press **Ctrl**+**End** to see the whole drawing.

Your diagram should look approximately like this:



Adding a Stream Table

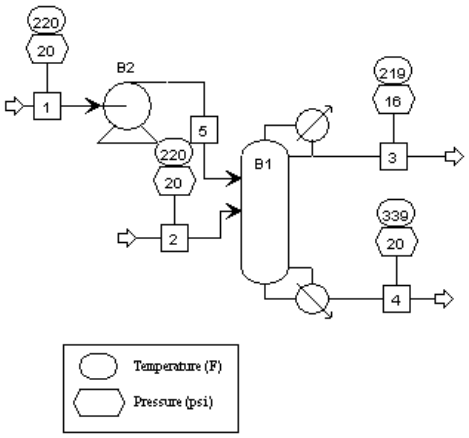
Process Flowsheet drawings frequently include a table of stream results (the heat and material balance table, or birdcage). To generate this table:

1. On the **Flowsheet | Modify** tab of the ribbon, click **Display Options** and ensure **Annotation** is selected.
2. Select **Results Summary | Streams** from the Navigation Pane.

   The **Results Summary - Streams** sheet appears with data from all streams displayed.
3. Click **Stream Table** to place the table on your diagram.
4. Click the **Main Flowsheet** tab in the workspace area to return to your flowsheet.

A birdcage-style stream table appears in the Flowsheet showing the stream results from the simulation:

Methylcyclohexane Recovery Process					
Stream ID		1	2	3	4
Temperature	F	220.0	220.0	218.8	338.7
Pressure	psi	20.00	20.00	16.00	20.20
Vapor Frac		0.000	0.000	0.000	0.000
Mole Flow	lbmol/hr	400.000	1800.000	200.000	2000.000
Mass Flow	lb/hr	38065.736	169403.472	19619.140	187850.068
Volume Flow	cuft/hr	827.446	2689.192	450.904	3291.453
Enthalpy	MMBtu/hr	-12.702	-107.917	-14.711	-93.888
Mole Flow	lbmol/hr				
TOLUENE		200.000		2.861	197.139
PHENOL			1800.000	0.291	1799.709
MCH		200.000		196.847	3.153
Mole Frac					
TOLUENE		0.500		0.014	0.099
PHENOL			1.000	0.001	0.900
MCH		0.500		0.984	0.002
*** VAPOR PHASE ***					
Density					
Viscosity					
*** LIQUID PHASE ***					
Density	lb/cuft	46.004	62.994	43.511	57.072
Viscosity	cP	0.288	1.021	0.324	0.442
Surface Ten	dyne/cm	16.805	31.995	14.903	23.580



Note: The table is scaled for printing.

You can zoom in on various parts of the diagram by enclosing an area and selecting **Zoom In** from the shortcut menu. See the directions below.

To Zoom in on Part of the Diagram

1. Drag the cursor (clicking and holding) across the area you would like to magnify.
2. When you have enclosed the area, release the cursor. It will be surrounded by a box.
3. With the cursor in the selected region, right-click in the background (not on any of the displayed objects) to display the shortcut menu.
4. From the shortcut menu, select **Zoom In**.

Adding Text

Add a title to the flowsheet using tools on the **Flowsheet** tabs of the ribbon.

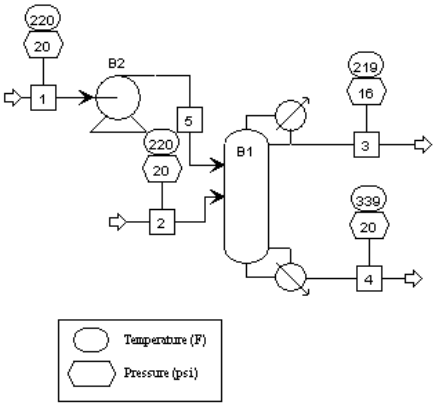
To Add Text

1. Click the **Flowsheet | Format** tab on the ribbon.
2. In **Shapes**, click  .
3. Move the cursor to an appropriate spot for the text and left-click.
   A rectangular box with a blinking cursor appears.
4. Type **Methylcyclohexane Recovery Column**, then click outside the rectangular box.
5. Select the title. Change the font size to **28** using the **Font Size** list in **Font**.
6. Click the title and hold the mouse button down until the cursor changes shape, then drag the title anywhere you like.
7. Click the **View** tab and select **Zoom to Fit**.

The final diagram looks like something like this:

Methylcyclohexane Recovery Column

Methylcyclohexane Recovery Process					
Stream ID		1	2	3	4
Temperature	F	220.0	220.0	218.8	338.7
Pressure	psi	20.00	20.00	16.00	20.20
Vapor Frac		0.000	0.000	0.000	0.000
Mole Flow	lbmol/hr	400.000	1800.000	200.000	2000.000
Mass Flow	lb/hr	38065.736	169403.472	19619.140	187850.068
Volume Flow	cuft/hr	827.446	2689.192	450.904	3291.453
Enthalpy	MMBtu/hr	-12.702	-107.917	-14.711	-93.888
Mole Flow	lbmol/hr				
TOLUENE		200.000		2.861	197.139
PHENOL			1800.000	0.291	1799.709
MCH		200.000		196.847	3.153
Mole Frac					
TOLUENE		0.500		0.014	0.099
PHENOL			1.000	0.001	0.900
MCH		0.500		0.984	0.002
*** VAPOR PHASE ***					
Density					
Viscosity					
*** LIQUID PHASE ***					
Density	lb/cuft	46.004	62.994	43.511	57.072
Viscosity	cP	0.288	1.021	0.324	0.442
Surface Ten	dyne/cm	16.805	31.995	14.903	23.580



Adding a Molecular Structure Symbol

A molecular structure shows the graphical structure of a component. Attaching molecular structure symbols to the process flowsheet can help you identify the streams. In Aspen Plus, you use the Molecule Editor to edit the graphical molecule structure for pure components. To add the molecule symbol for MCH to the flowsheet:

To Copy the Molecule Symbol of MCH From the Molecule Editor

1 Click the **Properties** bar on the Navigation Pane to enter the Properties environment.

The Flowsheet disappears in the Properties environment.

2 On the Navigation Pane, expand **Components | Molecular Structure** and click **MCH**.

The **Molecular Structure - MCH | General** sheet appears.

3 Click the **Structure** tab on the **Molecular Structure - MCH** form to display the graphical structure of MCH.

4 Click **Draw/Import/Edit** beside the graphic.

The **Molecule Editor** window appears.

5 At the top of the panel shown on the left side of the window, click  .

6 Drag a rectangle around the graphical structure for MCH to select the entire drawing.

7 Click  on the menu to copy the drawing to the clipboard.

8 Close the **Molecule Editor** window.

To Paste the Molecular Structure of MCH to the Process Flowsheet

1 Click the **Simulation** bar on the Navigation Pane to enter the Simulation environment. Then click the **Main Flowsheet** tab in the workspace.

2 Click the right mouse button on any blank area on the flowsheet to display the shortcut menu.

3 Select **Paste**.

The molecular structure of MCH is pasted to the process flowsheet.

4 Select this symbol and drag it near Stream 1 to show the MCH feed stream.

Note: You can paste any OLE object in this way (any object that you can paste into other common Windows programs).

Printing a Process Flow Diagram

Before you print, make sure that your printer is set up correctly. For more information on printing options, see the online help topic **Using Aspen Plus | Doing More with Simulations | Printing**.

To Print the Process Flowsheet

1 Open the Flowsheet.

2 From the ribbon, click **File**. Click **Print** in the **File** menu.

   The **Print** dialog box appears asking you where you want the output directed.

3 Select the appropriate printer and click **OK**.

Exiting Aspen Plus

1 Select **File | Exit** from the ribbon.

   The **Aspen Plus** dialog box appears.

2 Click **Yes** to save the simulation.

6 Estimating Physical Properties for a Non-Databank Component

This chapter guides you through the procedure for estimating physical properties for a component that is not present in the Aspen Plus databank.

You will use a known molecular structure and known properties of Thiazole to provide Aspen Plus with a starting point for estimating missing properties.

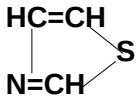
Allow about 30 minutes for this simulation.

Thiazole Physical Property Data

In this simulation, you are dealing with a process involving Thiazole and water, among other components.

Thiazole (C_3H_3NS) is not in the Aspen Plus databank. The following information is available from various sources:

Molecular structure for Thiazole:



Molecular weight: 85

Normal boiling point: 116.8 °C

Vapor pressure correlation:

$$\ln p_i^{oL} = 16.445 - 3281.0/(T+216.255)$$

For p_i^{oL} in mmHg, T in °C for 69 °C < T < 118°C

By checking the reference manual *Aspen Plus Physical Property Methods and Models*, Chapter 3 (in the online help) you see that you do not have data for all the required pure component property parameters for Thiazole.

You are missing data for the following property parameters (required for calculating enthalpies and densities):

Parameter	Description
TC	Critical temperature
PC	Critical pressure
CPIG	Ideal gas heat capacity coefficients
DHFORM	Heat of formation
DGFORM	Gibbs free energy formation
DHVLWT	Watson heat-of-vaporization coefficients
VC	Critical volume
ZC	Critical compressibility factor

Run a Property Estimation simulation in Aspen Plus to estimate the missing property parameters for Thiazole required to run your simulation.

Starting Aspen Plus

1. From your desktop, select **Start** and then select **Programs**.
2. Select **AspenTech | Process Modeling <version> | Aspen Plus | Aspen Plus <version>**.

   The Aspen Plus main window appears.
3. From the ribbon, select **File** and click **New**.

   The **New** dialog box appears.

Creating a Property Estimation Simulation

Use the **New** dialog box to specify the template for the new simulation.

1. From the **New** dialog box, select **Chemical Processes** from the panel on the left side.
2. Click the **Chemicals with English Units** template.
3. Click **Create**.

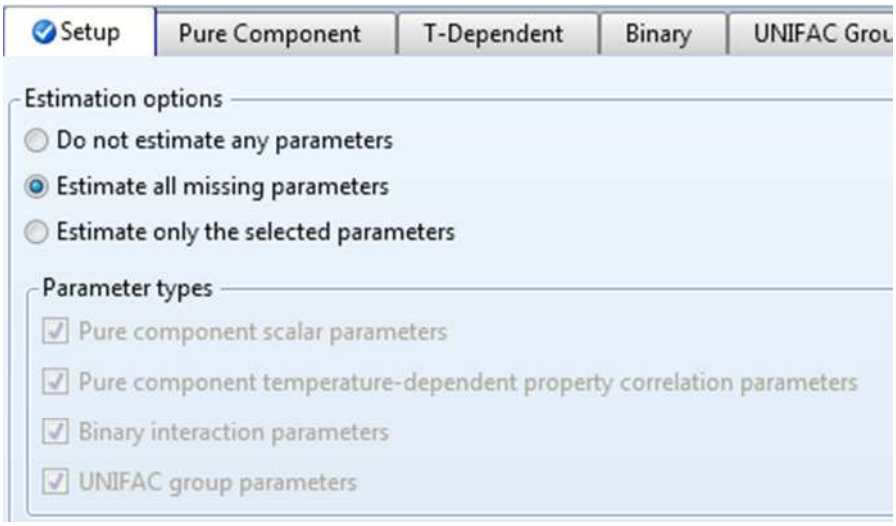
   The template is loaded in **Properties** environment.
4. On the **Home** tab of the ribbon, click **Estimation** in **Run Mode**.

   The **Estimation - Input | Setup** sheet appears.

There is no need to build a process flowsheet for a Property Estimation run. First enter a title for the simulation. Then define a new component with the name **thiazole** and tell Aspen Plus to estimate all missing properties. Then enter the molecular structure of Thiazole and all known properties. Then run the estimation.

Specifying Properties to Estimate

The option **Estimate all missing parameters** is selected.



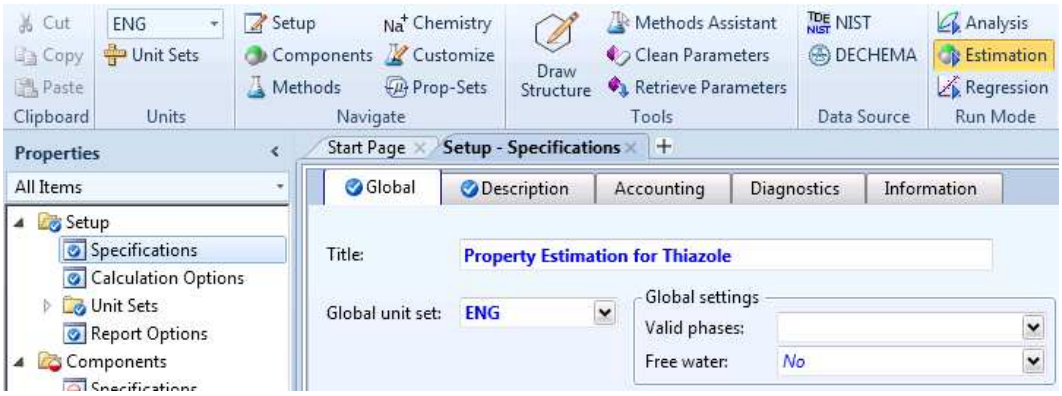
The other sheets on this form allow you to select specific estimation methods for each property if you do not wish to use the default methods. For this example, the defaults are adequate.

Next, enter the molecular structure of Thiazole.

Entering a Title

1. Expand the **Setup** folder on the Navigation Pane and click **Specifications**.

   The **Setup - Specifications | Global** sheet appears.
2. In the **Title** field, type **Property Estimation for Thiazole**.



Next, define a component called THIAZOLE.

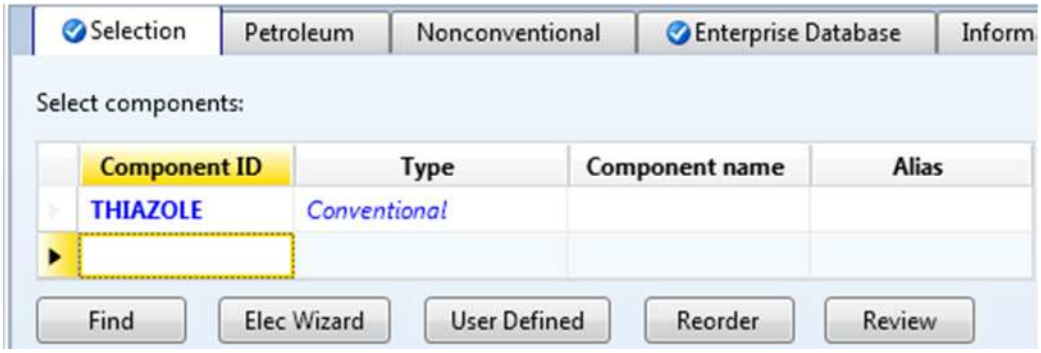
Entering Components Information

1 From the Navigation Pane, expand the **Components** and click **Specifications**.

The **Components - Specifications | Selection** sheet appears.

2 In the first line of the **Component ID** column, enter **THIAZOLE**.

Because THIAZOLE is not in the Aspen Plus databank, do not fill in the **Component name** or **Alias** columns.



Next, tell Aspen Plus to estimate all missing properties.

Entering Molecular Structure

To Enter the Molecular Structure Information for Thiazole

1 Expand the **Components | Molecular Structure** folder on the Navigation Pane, click **THIAZOLE**.

The **Molecular Structure - THIAZOLE | General** sheet appears.

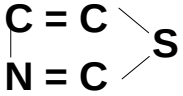
Note: You can define the molecular structure by using the **General** Method which is based on individual atoms and bonds, or by using the **Functional Group** method in which you indicate the functional groups specific to a particular estimation method, or by drawing the structure. This example explains how to draw the structure.

2 Click the **Structure** tab to open the **Molecular Structure - THIAZOLE | Structure** sheet.

3 Click **Draw/Import/Edit**.

The **Molecule Editor** dialog box appears.

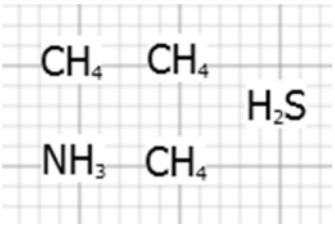
Sketch the structure of Thiazole in the **Molecule Editor** window, ignoring hydrogen atoms:



4 Select the atoms and place the atoms on the drawing workspace. Click **C** under **Atoms**, then click three times in the drawing workspace to create 3 carbon atoms. Follow the same steps to place a nitrogen atom and a sulfur atom.

5 Click the arrow icon (**Select**) above **Bonds and Charges**. Click an atom and drag it to a proper place in the workspace.

The atoms should be placed as below.

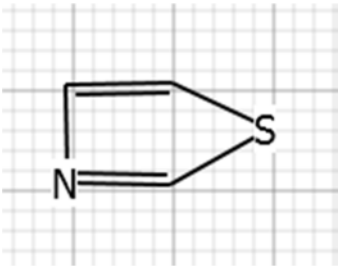


6 Select the bonds and connect the atoms. Click **Single Bond** under **Bonds and Charges**, click the carbon atom on the top left, hold the left mouse button and move the cursor to the nitrogen atom below the carbon atom you have selected. Release the mouse button after a single line appears. After the atoms are connected, the numbers of the hydrogen will be recalculated.

Follow the same steps to connect the sulfur atom with the two carbon atoms next to it.

7 Click **Double Bond** and connect the 2 carbon atoms in the top line, as well as the nitrogen atom and carbon atom in the bottom line.

The completed molecule structure should be the same as below.



8 Close the **Molecule Editor** window. When prompted whether to save the structure, click Yes. The graphical structure is displayed on the **Molecular Structure - THIAZOLE | Structure** sheet.

9 Click **Calculate Bonds**.

The mark is displayed on the **General** and **Formula** tabs, indicating these tabs are completed. Aspen Plus automatically uses the bond data from the drawn structure to fill in these sheets.

Next, enter the known property data for thiazole.

Entering Property Data

The molecular structure information is sufficient for Aspen Plus to estimate properties. However, entering all available data will improve the accuracy of the Aspen Plus estimation.

To Enter Pure Component Boiling Point and Molecular Weight for Thiazole

1 Expand the **Methods | Parameters** folder on the Navigation Pane and click **Pure Components**.

The **Pure Components** object manager appears.

2 Click **New**.

3 In the **New Pure Component Parameters** dialog box, verify **Scalar** is selected.

4 Enter the new name **TBMW** (for boiling point and molecular weight) and click **OK**.

The **Pure Components - TBMW | Input** sheet appears.

5 In the **Component** field, click  and select **THIAZOLE**.

6 Click the **Parameters** field, and select **TB** (normal boiling point).

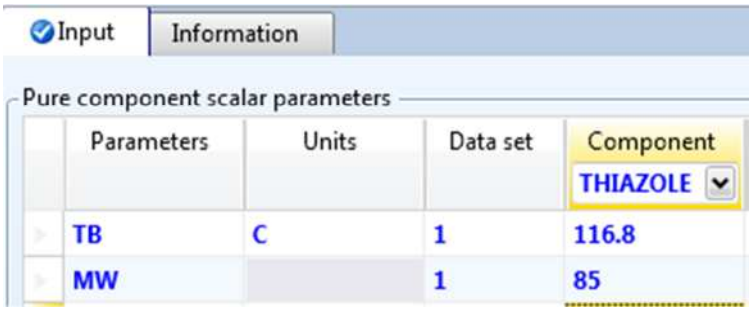
7 Click the **Units** field, and select **C** to express the boiling point in degrees Celsius.

8 In the fourth column (under the **Component** field) enter **116.8**.

9 Click the second cell under the **Parameters** column, and select **MW** (molecular weight).

10 In the fourth column, enter **85**.

You have entered the pure component property data for Thiazole.



Next specify the coefficients for the Antoine vapor pressure correlation.

To Enter Antoine Vapor Pressure Correlation Coefficients

1 Click **Methods | Parameters | Pure Components** on the Navigation Page.

The object manager appears. You can see that you have filled your TBMW parameters with scalar data.

2 Click **New.**

3 In the **New Pure Component Parameters** dialog box, select **T-dependent correlation**. A tree-style of choices appears in the box below the three pure component parameter types.

4 Under **Liquid vapor pressure**, select **PLXANT-1** for the Antoine vapor pressure correlation.

5 Click **OK**.

The **Pure Components - PLXANT-1 | Input** sheet appears.

6 Click the **Components** field, select **THIAZOLE**.

The Antoine vapor pressure correlation (also given above) is:

$$\ln p_i^{oL} = 16.445 - 3281.0/(T+216.255)$$

for p_i^{oL} in mmHg, T in °C for 69 °C < T < 118°C.

You can get help on specifying the coefficients by clicking **PLXANT** in the **Parameter** field near the top of this sheet and then press **F1**. Follow the link to **General Pure Component Liquid Vapor Pressure**.

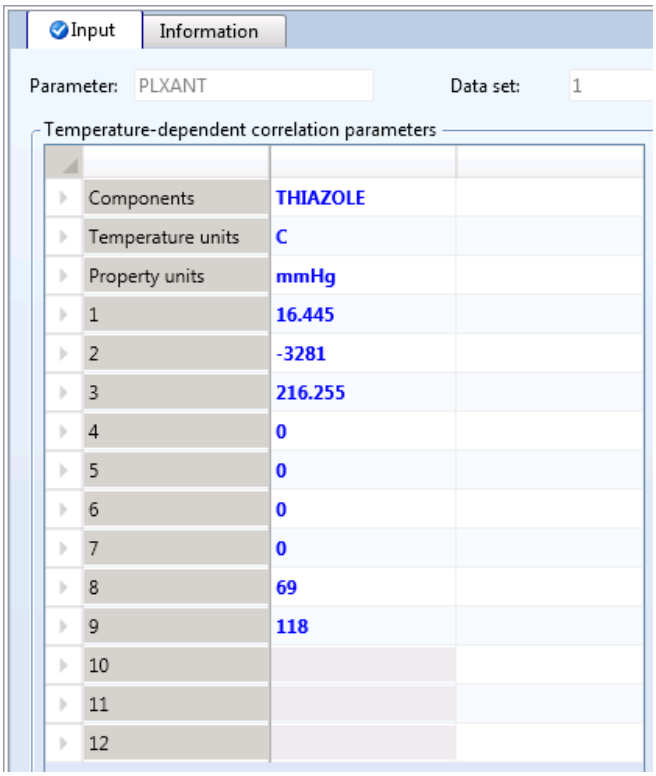
7 Click the **Temperature units** field, select **C**.

8 Click the **Property units** field, select **mmHg**.

9 Enter the Antoine coefficients for Thiazole in the fields numbered 1 through 9.

Field	Coefficient
1	16.445
2	-3281
3	216.255
4	0
5	0
6	0
7	0
8	69
9	118

You have completed the **Pure Components - PLXANT-1 | Input** sheet:



You have entered all available property data for thiazole and are now ready to run the property constant estimation system (PCES).

Running a Property Constant Estimation (PCES)

Click  in the **Home** tab of the ribbon or press **F5** to run the estimation.

As the run executes, status messages display in the **Control Panel**. Click **Control Panel** to see the runtime messages. The message *Results Available with Warnings* appears in the Status bar at the bottom of the main window. In this example. Ignore these warnings since you did not use functional groups in your structure specification.

Examining Property Constant Estimation Results

Examine the results of your PCES simulation. View the Pure Component and T-dependent properties estimated by Aspen Plus.

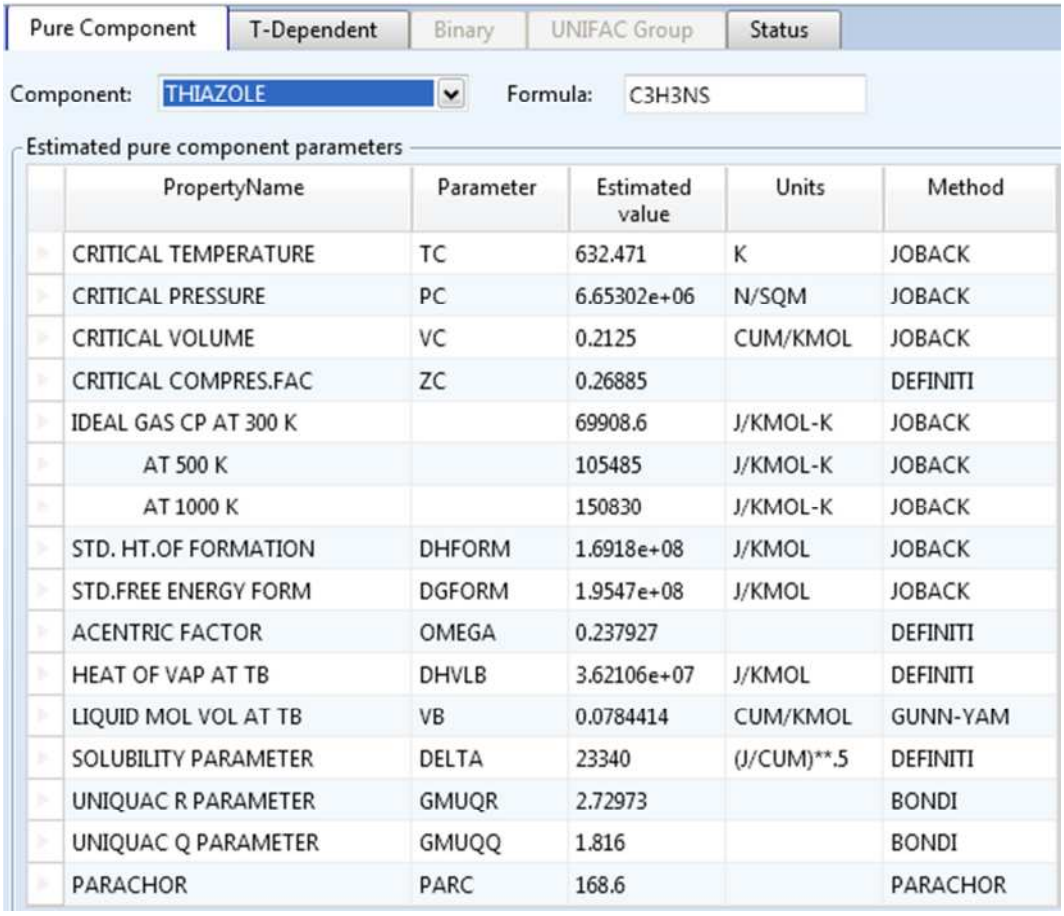
To Examine PCES Results

1 On the Navigation Pane, click **Results Summary | Run Status**.

A summary sheet appears indicating that the calculations were completed with warnings.

2 Navigate to **Estimation | Results**.

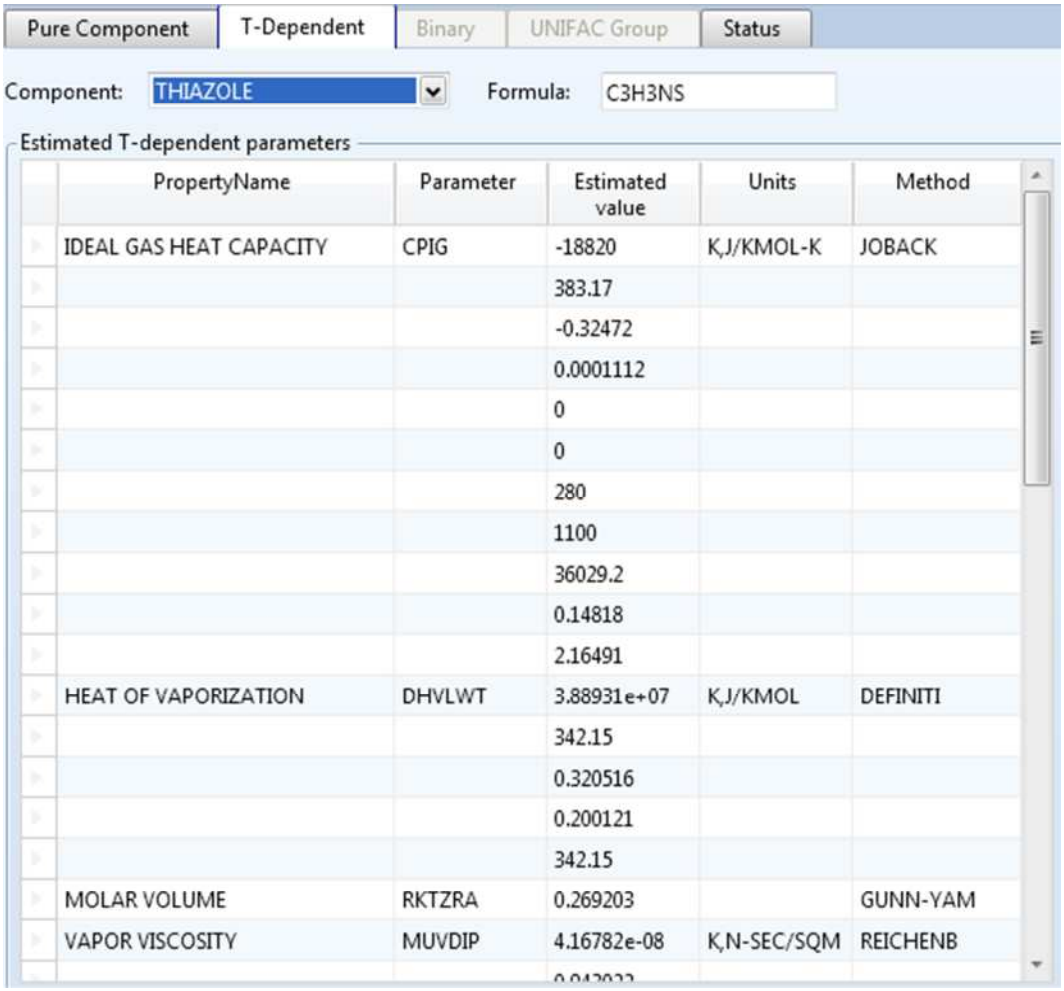
The **Estimation - Results | Pure Component** sheet appears, with the estimated pure component properties for Thiazole. The property name, abbreviation, estimated value, units, and method used for estimation are tabulated.



PropertyName	Parameter	Estimated value	Units	Method
CRITICAL TEMPERATURE	TC	632.471	K	JOBACK
CRITICAL PRESSURE	PC	6.65302e+06	N/SQM	JOBACK
CRITICAL VOLUME	VC	0.2125	CUM/KMOL	JOBACK
CRITICAL COMPRES.FAC	ZC	0.26885		DEFINITI
IDEAL GAS CP AT 300 K		69908.6	J/KMOL-K	JOBACK
AT 500 K		105485	J/KMOL-K	JOBACK
AT 1000 K		150830	J/KMOL-K	JOBACK
STD. HT.OF FORMATION	DHFORM	1.6918e+08	J/KMOL	JOBACK
STD.FREE ENERGY FORM	DGFORM	1.9547e+08	J/KMOL	JOBACK
ACENTRIC FACTOR	OMEGA	0.237927		DEFINITI
HEAT OF VAP AT TB	DHVLB	3.62106e+07	J/KMOL	DEFINITI
LIQUID MOL VOL AT TB	VB	0.0784414	CUM/KMOL	GUNN-YAM
SOLUBILITY PARAMETER	DELTA	23340	(J/CUM)**.5	DEFINITI
UNIQUAC R PARAMETER	GMUQR	2.72973		BONDI
UNIQUAC Q PARAMETER	GMUQQ	1.816		BONDI
PARACHOR	PARC	168.6		PARACHOR

3 Click the **T-Dependent** tab.

The T-Dependent sheet appears with estimated coefficients for polynomials that model the temperature dependence of the listed properties. The property name, abbreviation, list of coefficients, units, and method are tabulated:



PropertyName	Parameter	Estimated value	Units	Method
IDEAL GAS HEAT CAPACITY	CPIG	-18820	K,J/KMOL-K	JOBACK
		383.17		
		-0.32472		
		0.0001112		
		0		
		0		
		280		
		1100		
		36029.2		
		0.14818		
		2.16491		
HEAT OF VAPORIZATION	DHVLWT	3.88931e+07	K,J/KMOL	DEFINITI
		342.15		
		0.320516		
		0.200121		
		342.15		
MOLAR VOLUME	RKTZRA	0.269203		GUNN-YAM
VAPOR VISCOSITY	MUVDIP	4.16782e-08	K,N-SEC/SQM	REICHENB

Creating and Using a Property Backup File

Save this property estimation as a backup file (.bkp) that you can import into a flowsheet simulation that uses thiazole.

To Save a Backup File

1. Select **File | Save As** from the ribbon.
2. Select **Aspen Plus Backup** in the list on the left. The **Save As** dialog box appears.
3. In the **File Name** field, enter **thiazole**.
4. Click **Save**.
5. An Aspen Plus dialog box appears, informing you that this file format does not support restarting calculations from previous results, and asking whether you want to also save an Aspen Plus Document (*.apw). Since you only need the final results, click **No**.

Next, try using your backup file to import thiazole data into flash.apw.

To Import a Backup File

Run the Flash simulation with methanol, water, and thiazole in Stream 1. Follow these steps.

1 Click **File | Open** and select **Flash.apw** from your working folder. Click **Yes** to close the thiazole estimation.

Note: You don't have to close the current run before opening a new run. If you click **No**, you will have two Aspen Plus applications running at the same time, each with one open simulation (Aspen Plus cannot open multiple simulations).

2 Select **File | Import** from the ribbon, and select **File**. In the **Import** dialog box, browse and select **thiazole.bkp**. Click **Open**.

Note: You cannot import an Aspen Plus document file (.apw) into another simulation.

3 A dialog box appears informing you that importing a simulation requires fully loading results for the current simulation. Click OK.

The **Resolve ID Conflicts** dialog box appears. The only conflicts are units sets and the NRTL property method.

4 Click the NRTL line, then **Merge**.

5 Click the first unit set, then hold the **Shift** key and click the last one to select all three unit sets. Click **Ignore** to ignore the unit sets from the imported file. Then click **OK**.

6 Click the **Properties** bar on the Navigation Pane to enter the **Properties** environment.

7 On the Navigation Pane, click **Estimation | Input**. Select **Do not estimate any parameters** since the thiazole parameters have already been estimated.

8 Click the **Simulation** bar on the Navigation Pane to enter the **Simulation** environment.

9 On the Navigation Pane, click **Streams | 1 | Input** and then in the **Composition** area of the **Specifications** sheet, type **50** for the mole flow of the component thiazole which is now listed along with methanol and water.

10 Press **F5** to run the simulation with thiazole in Stream 1.

Exiting Aspen Plus

1 Select **File | Exit** from the ribbon.

An **Aspen Plus** dialog box appears.

2 Click **No** to preserve the original Flash simulation (without thiazole).

7 Analyzing Properties

Before starting a simulation study, it is important to understand the physical property and phase equilibrium behavior of the fluids in your process, and to confirm that the behavior predicted by the property models and data you are using is reasonable.

In this chapter you will use the interactive property analysis features in Aspen Plus to obtain a binary T-xy diagram for the acetone-chloroform system, using the NRTL activity coefficient model with parameters from the built-in binary pair databank. Then you will check your results against literature data.

Allow about 20 minutes for this simulation.

Starting Aspen Plus

1. From your desktop, select **Start** and then select **Programs**.
2. Select **AspenTech | Process Modeling <version> | Aspen Plus | Aspen Plus <version>**.

   The **Start Using Aspen Plus** window appears.
3. Click **File** on the ribbon and select **New**.

   The **New** dialog box appears.
4. Select **Chemical Processes** from the panel on the left side. Click the **Chemicals with English Units** template.
5. Click **Create**.
6. Verify that **Analysis** is selected in **Run Mode** on the **Home** tab of the ribbon.

The Aspen Plus main window appears. Aspen Plus starts a new simulation with the default name, Simulation 1 in the **Properties** environment.

Entering Components and Properties

You do not need a process flowsheet to perform a property analysis. You require information only about chemical species and physical properties.

1 In the Navigation Pane area, click **Setup | Specifications**.

The **Setup - Specifications | Global** sheet appears.

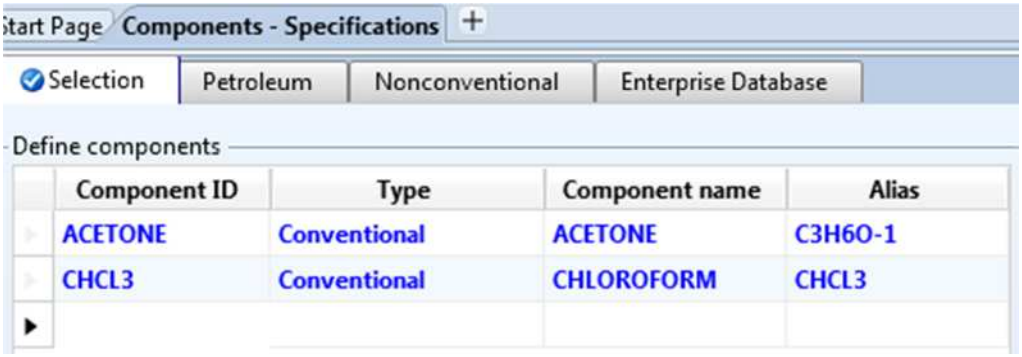
2 Enter a title if you wish.

Select a units set consistent with the literature data you will use for comparison.

3 From the ribbon, on the **Home** tab, in **Units**, click  and select **METCBAR** for METric units with Celsius for temperature and BAR for pressure.

4 On the **Components - Specifications | Selection** sheet, type **ACETONE** and press **Enter** on the keyboard.

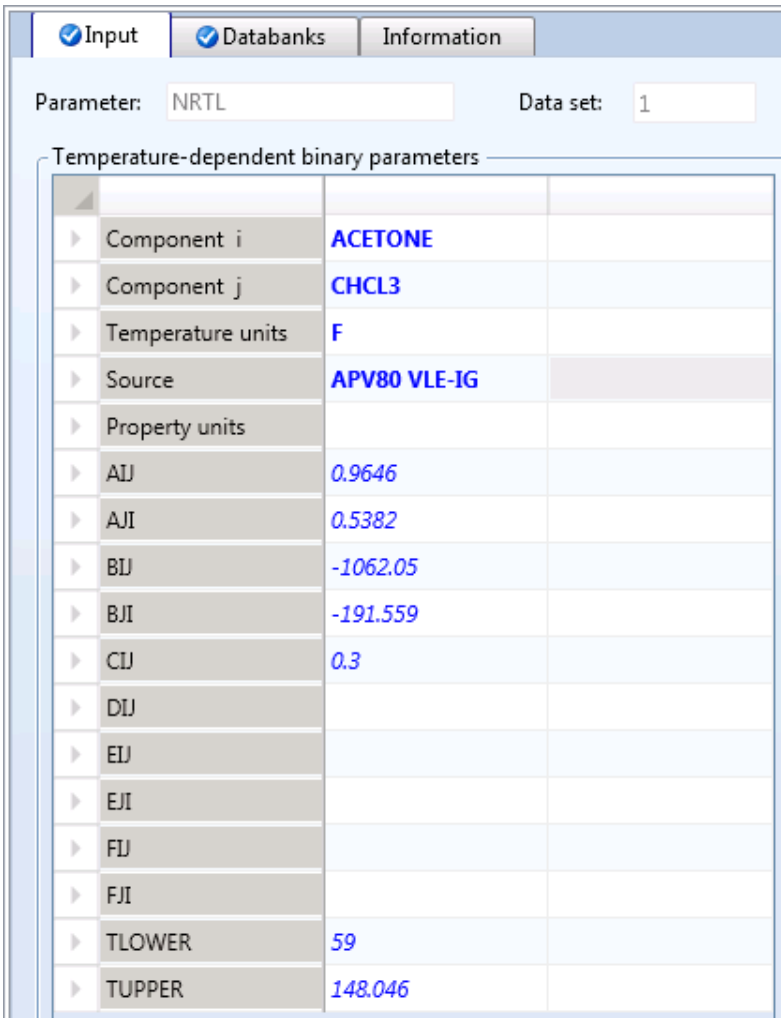
5 In the second line under the **Component ID** field, type **CHCL3** for chloroform and press **Enter** on the keyboard. A dialog box appears asking about updating parameters for the newly added component. Click **Yes**.



Aspen Plus matches the component IDs against the Aspen Plus databanks and fills in the information for acetone and chloroform on the sheet.

6 Click  .

The **Binary Interaction - NRTL-1 (T-DEPENDENT) | Input** sheet appears:

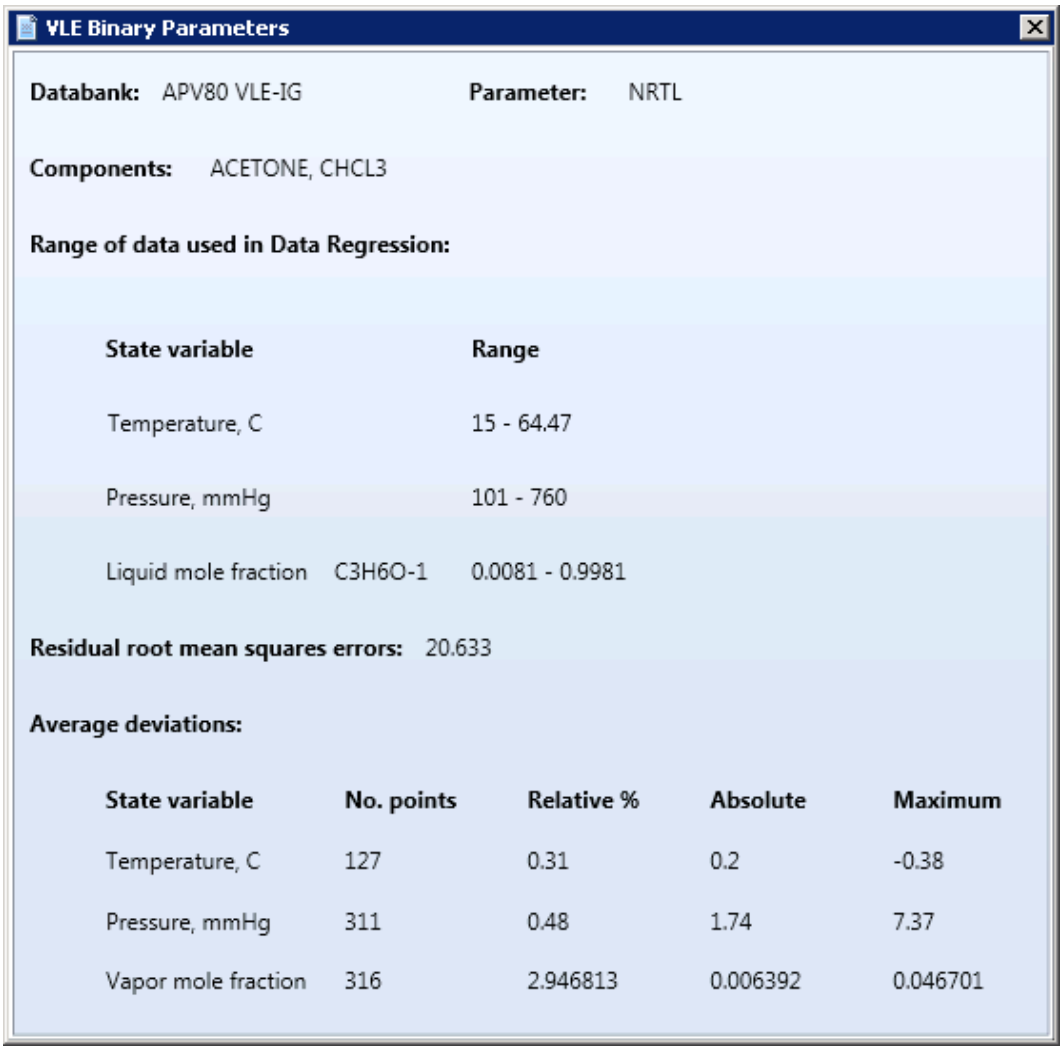


This sheet displays the default binary parameters for acetone-chloroform retrieved from the Aspen Plus databanks. These parameters were determined from literature data for this binary system between 59 F and 148.046 F.

Examine additional information on the range of data used and the quality of the fit.

7 Click **APV80 VLE-IG** in the form. Click **Regression Info**.

Note: If you are using the legacy databank system, the **Regression Info** button will not be present. In this case, click one of the fields containing a numerical value and then press F1. The same information shown below will appear but in a different format.



VLE Binary Parameters

Databank: APV80 VLE-IG **Parameter:** NRTL

Components: ACETONE, CHCL3

Range of data used in Data Regression:

State variable		Range
Temperature, C		15 - 64.47
Pressure, mmHg		101 - 760
Liquid mole fraction	C3H6O-1	0.0081 - 0.9981

Residual root mean squares errors: 20.633

Average deviations:

State variable	No. points	Relative %	Absolute	Maximum
Temperature, C	127	0.31	0.2	-0.38
Pressure, mmHg	311	0.48	1.74	7.37
Vapor mole fraction	316	2.946813	0.006392	0.046701

Review the help to confirm that the default parameters are appropriate for your analysis.

8 Close the window.

Generating a Txy Diagram

You can use the Aspen Plus analysis capability before input specifications are complete, though in this case, they are complete. Note the *Required Properties Input Complete* message on the status bar.

Aspen Plus can generate four types of property analysis: pure, binary, residue, and stream. However, with the given input, only pure and binary analyses are available.

In this simulation, study VLE behavior of the acetone-chloroform binary system, so you can perform a binary analysis.

The relevant literature values are:

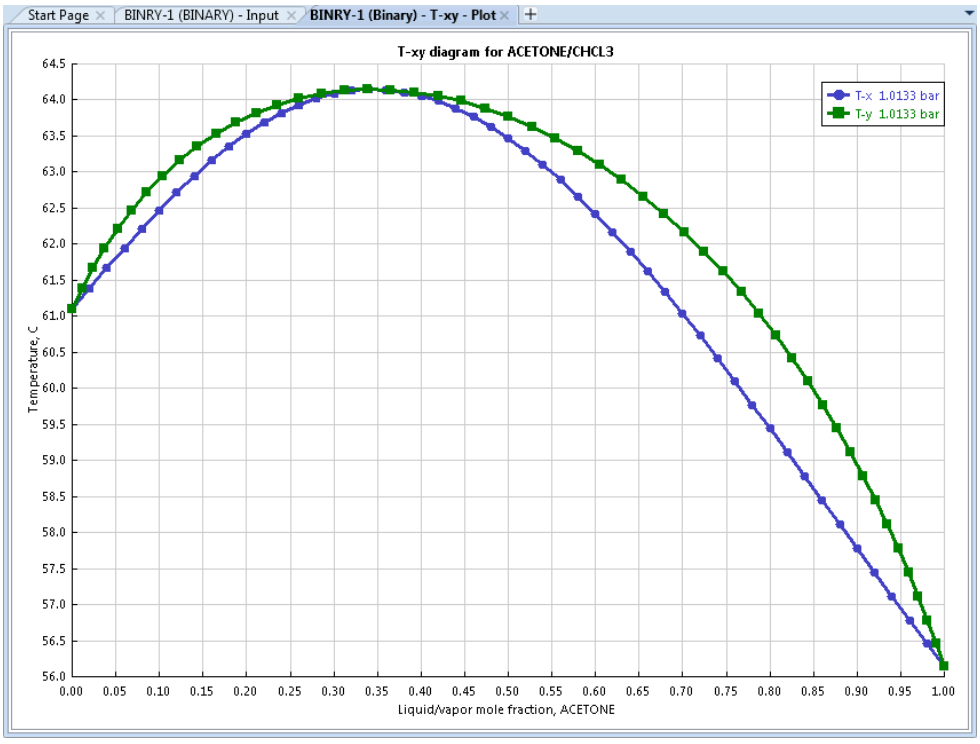
Acetone boiling point	56 °C

Chloroform boiling point	61 °C
Acetone-chloroform azeotrope	64.5 °C

(From *Mass-Transfer Operations*, Treybal, 3rd Ed., McGraw-Hill, p. 356, and from *Properties of Gases and Liquids*, Reid, Sherwood and Prausnitz, 3rd Ed., McGraw-Hill, Chapter 9.)

To Generate a Txy Diagram

1. From the ribbon, on the **Home** tab, click **Analysis | Binary**.
   The **BINRY-1 (BINARY) - Input | Binary Analysis** sheet appears.
2. In the **Analysis type** field, click  to view the types of analysis available.
   As the prompts indicate, Txy and Pxy analysis are used to study nonideality of vapor-liquid systems to check for azeotrope formation. Gibbs energy of mixing analysis is used to see if the system will form two liquid phases.
3. Select **Txy**.
   The fields on this sheet are filled with default options all of which are correct for this example.
4. Click **Run analysis** to apply the defaults and start the analysis.
   Calculations begin for the T-xy diagram. When the calculations are finished, a T-xy plot is automatically displayed, as shown in the following figure:



This plot indicates that this system contains an azeotrope at an acetone mole fraction of about 0.34 and a temperature of 64.2 °C (147.5 F). The

temperature of the azeotrope agrees with the literature value within 0.5%, so you could feel confident using the Aspen Plus default data in a simulation.

5 From the Navigation Pane, click **Analysis | BINRY-1 | Results**.

This shows the results in a tabular form. The table on the sheet shows that Aspen Plus has calculated activity coefficients (GAMMA) and K-values as well as temperature and composition. Use the horizontal and vertical scrollbars to see all the data. Several additional built-in plots are available in Aspen Plus.

To Generate an Activity Coefficient Plot

1 On the **Home** tab of the ribbon, in **Plot**, click the arrow beside the built-in plot library field to display all plot types.

2 Select **Custom.**

3 To plot activity coefficients versus mole fraction of acetone, in the **X Axis** field select **MOLEFRAC ACETONE**, and in the **Y Axis** area, select the checkboxes next to **LIQUID1 GAMMA ACETONE** and **LIQUID1 GAMMA CHCL3** and clear all other checkboxes. Click **OK**.

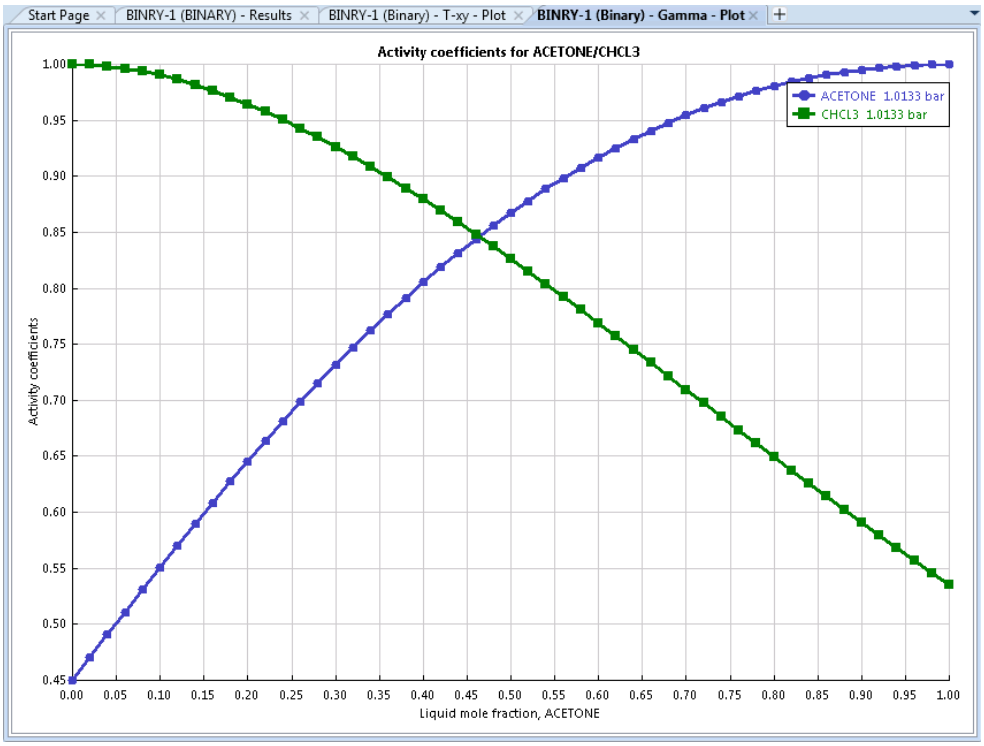
The activity coefficient plot appears.

4 In the **Plot | Format** tab of the ribbon, click **Y axis map**.

5 Click **Single Y Axis**, then click **OK**.

6 Right-click the label on the Y axis, then click **Edit**. Type the label **Activity coefficients**, then press **Enter**.

Now the plot is finished:



Note: The **Plot | Design** and **Plot | Format** tabs are shown on the ribbon when the plot window is active.

From this plot you can see the infinite dilution activity coefficients.

Exiting Aspen Plus

1 From the ribbon**,** select **File | Exit.**

2 In the **Aspen Plus** dialog box, click **No**.