

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** 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.
- 2** Specify the chemical components in the process. You can take these components from the Aspen Plus databanks, or you can define them.
- 3** Specify thermodynamic models to represent the physical properties of the components and mixtures in the process. These models are built into Aspen Plus.
- 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 Creating a Process Flow Diagram	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 users learn and use Aspen Plus.

Title	Content
Aspen Plus Getting Started Modeling Petroleum Processes	Tutorials covering the Aspen Plus features designed to handle petroleum
Aspen Plus Getting Started Modeling Processes with Solids	Tutorials covering the Aspen Plus features designed to handle solids

Title	Content
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 **Aspen Engineering Suite**, then **Aspen Plus <version>**, and then **Aspen Plus User Interface**.

The **Aspen Plus Startup** dialog box appears. Aspen Plus displays a dialog box whenever you must enter information or make a selection before proceeding.

- 3 Select **Blank Simulation**, then click **OK**.

If the **Connect to Engine** dialog box appears, see "[Connecting to the Aspen Plus Simulation Engine](#)" on page 93.

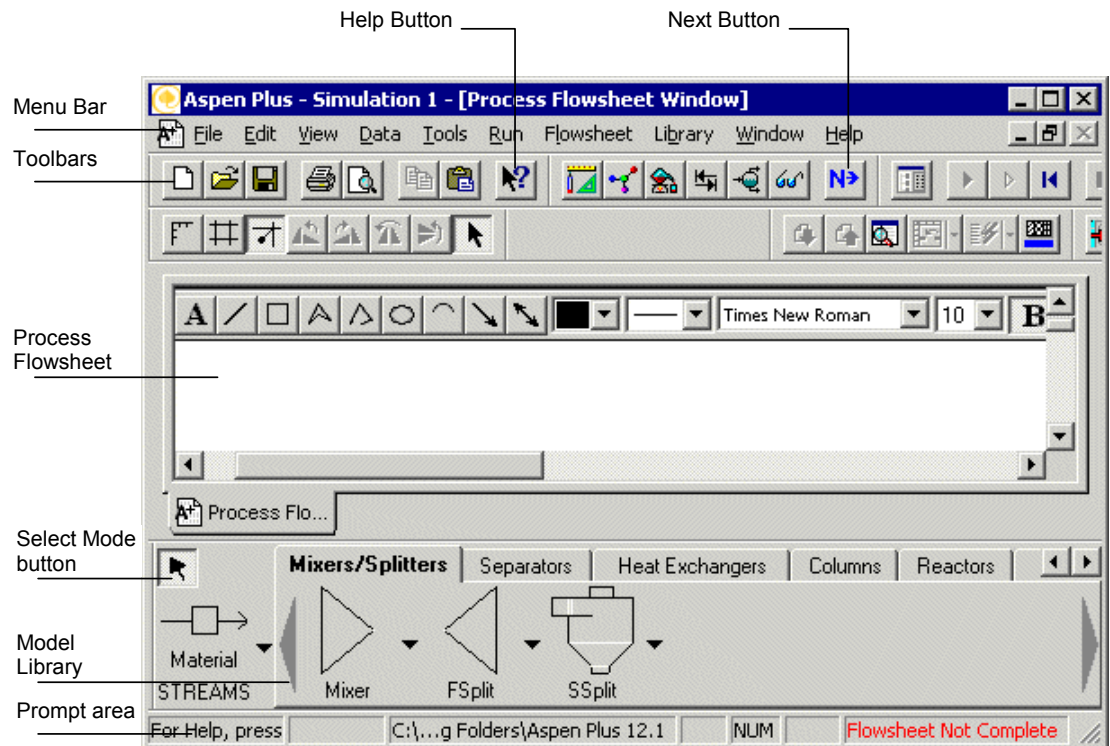
Note: To create a Windows desktop icon for Aspen Plus, right-click **Aspen Plus User Interface** via the **Start** menu, click **Copy**, then right-click on your desktop and select **Paste Shortcut**. Double-click the icon to start Aspen Plus.

The Aspen Plus Main Window

The Aspen Plus main window (shown below) appears when you start Aspen Plus. From the menu bar, select **Window** and then select **Workbook** to get the display style shown below. **Workbook** mode is used in all the examples in this book.

The Process Flowsheet Window appears automatically along with the Aspen Plus menu bar, various toolbars, and the Model Library.

Aspen Plus displays context-dependent definitions and information in the prompt area of the main window. Whenever you need information about the currently highlighted item, refer to the prompt area for guidance.



Opening a File

Open a file for an Aspen Plus simulation by either:

- 1 Double-clicking the file in Windows.
- 2 Selecting the **Open** command from the **File** menu in Aspen Plus.

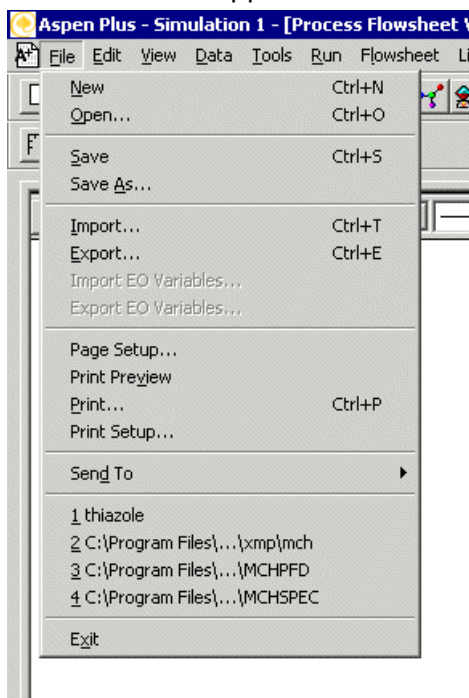
In this section, use the **Open** command on the **File** menu to open a partially completed Aspen Plus simulation stored in a backup file.

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 From the menu bar, select **File**.

The **File** menu appears:

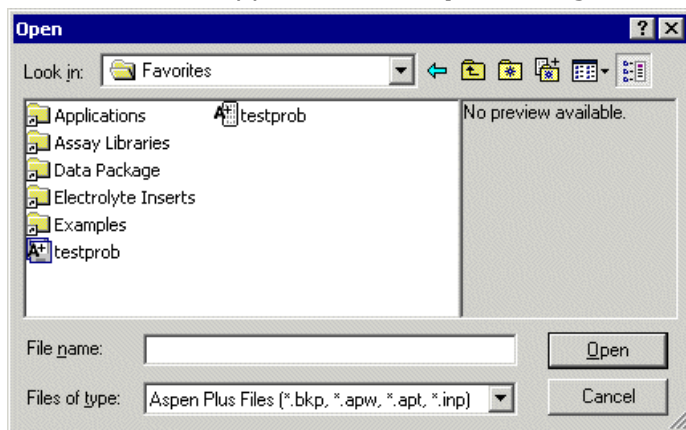


- 2 From the **File** menu, select **Open**.

The **Open** dialog box appears. Your default working directory appears in the **Look in** list.

- 3 Click .

A list of folders appears in the **Open** dialog box:



By default, the Favorites list contains five folders that are provided with Aspen Plus. The files in these folders are designed to assist in creating suitable simulation models in Aspen Plus.

Note: Add folders to the Favorites list by navigating to the appropriate

folder and clicking .

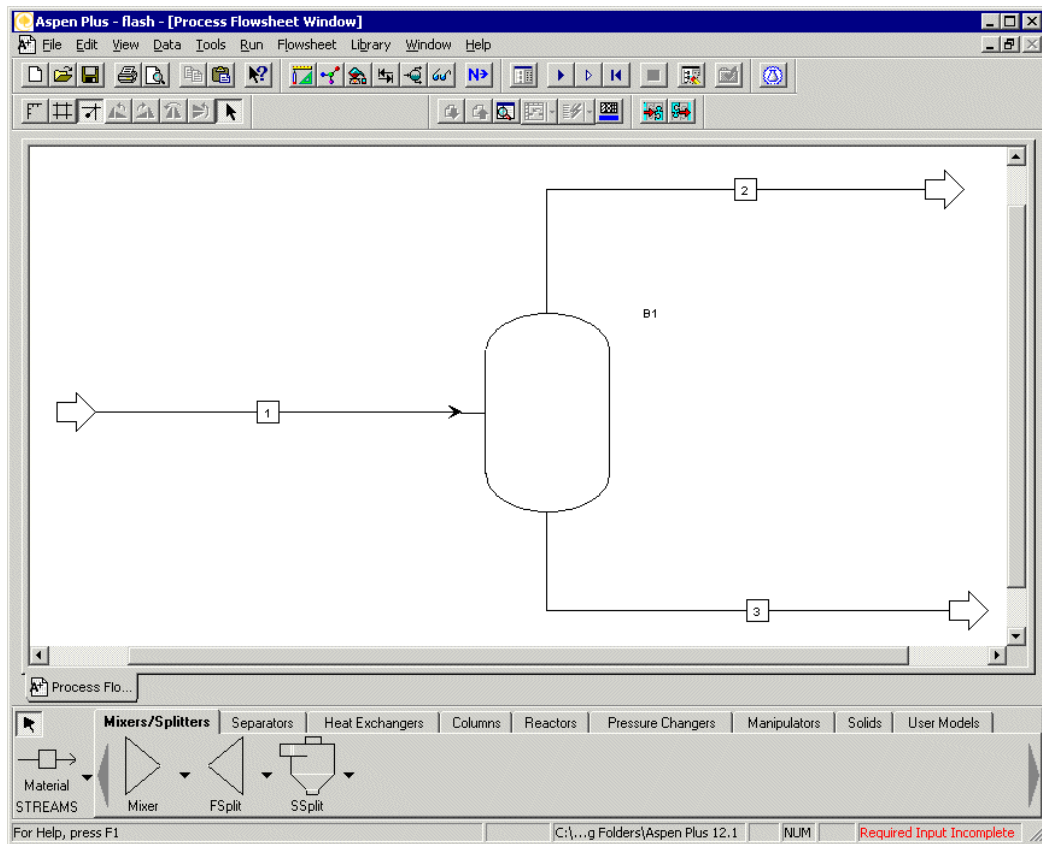
- 4 Double-click the **Examples** folder.
- 5 From the files list, select **flash.bkp** and click **Open**.
- 6 From the **Aspen Plus** dialog box, click **Yes** to close the current run before opening a new run.
- 7 If Aspen Plus prompts "Save changes to Simulation 1?", click **No**.

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.

Note: You don't have to close the current run before opening a new run. If you click **No** in step 6, you will have two Aspen Plus applications running at the same time, each with one open simulation (Aspen Plus cannot open multiple simulations).

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

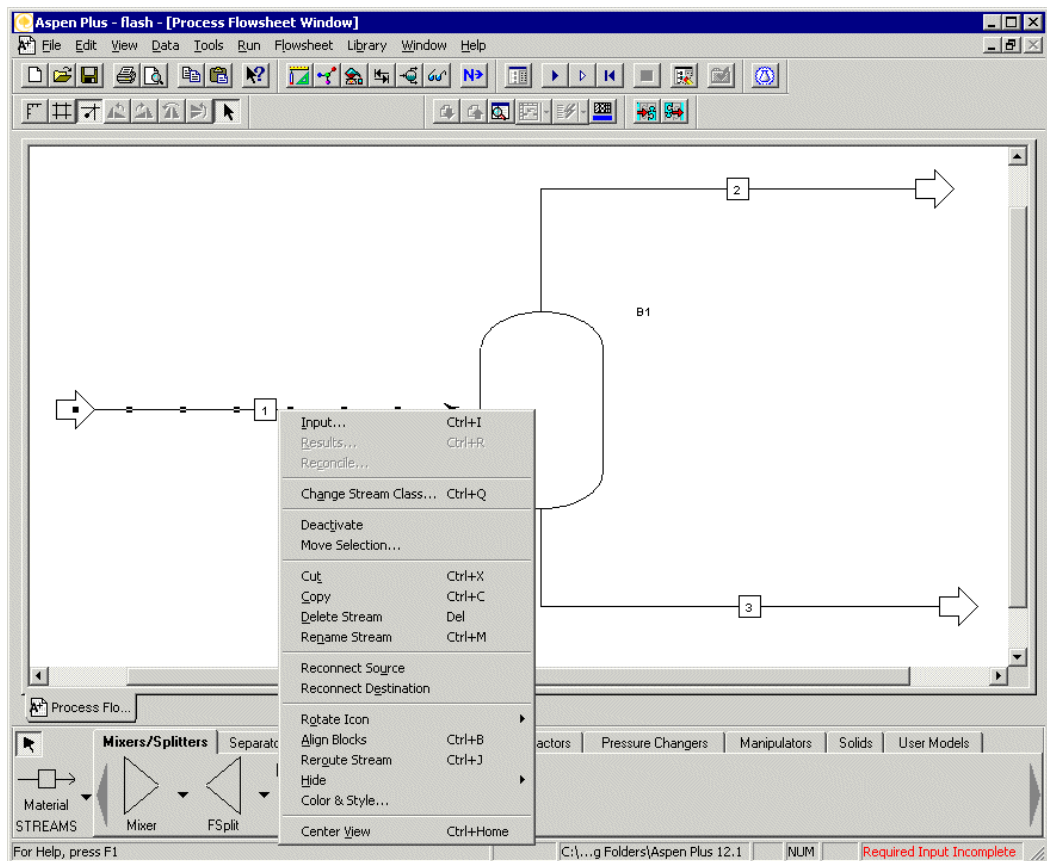
A shortcut menu of commands is available for the flowsheet objects.

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 Use the **Up** and **Down** arrow keys on your keyboard, to highlight the commands in the shortcut menu.


The prompts at the bottom of the main window change as you highlight each command.

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 a number of ways to access the input sheets:

- From the Aspen Plus menu bar, select **Data** and then select **Data Browser**, then use the Data Browser menu tree to navigate to the **Streams | 1 | Input | Specifications** 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 menus.

- From the Aspen Plus menu bar, select **Data | Streams**, then use the Data Browser menu tree to navigate to the **Streams | 1 | Input | Specifications** sheet.
- Click the streams button  in the Data Browser toolbar, then use the Data Browser menu tree to navigate to the **Streams | 1 | Input | Specifications** sheet.
- From the stream 1 shortcut menu, select **Input**.

To Open the Input Sheets for Stream 1

- 1 From the process flowsheet, select Stream 1, then click the right mouse button.
- 2 From the stream shortcut menu, select **Input**.

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

The **Stream 1 Input Specifications** sheet appears with the Data Browser menu tree in the left pane:


Error! Objects cannot be created from editing field codes.

Navigate from sheet to sheet by expanding the folders in the Data Browser menu tree and clicking the lowest level objects. For example, if you want to see the input sheet for Block B1, expand the Blocks folder and the B1 folder and click **Input**.

Navigate from window to window by clicking the Window Tabs. For example, if you want to go back to the Process Flowsheet, click its tab.

Using Help

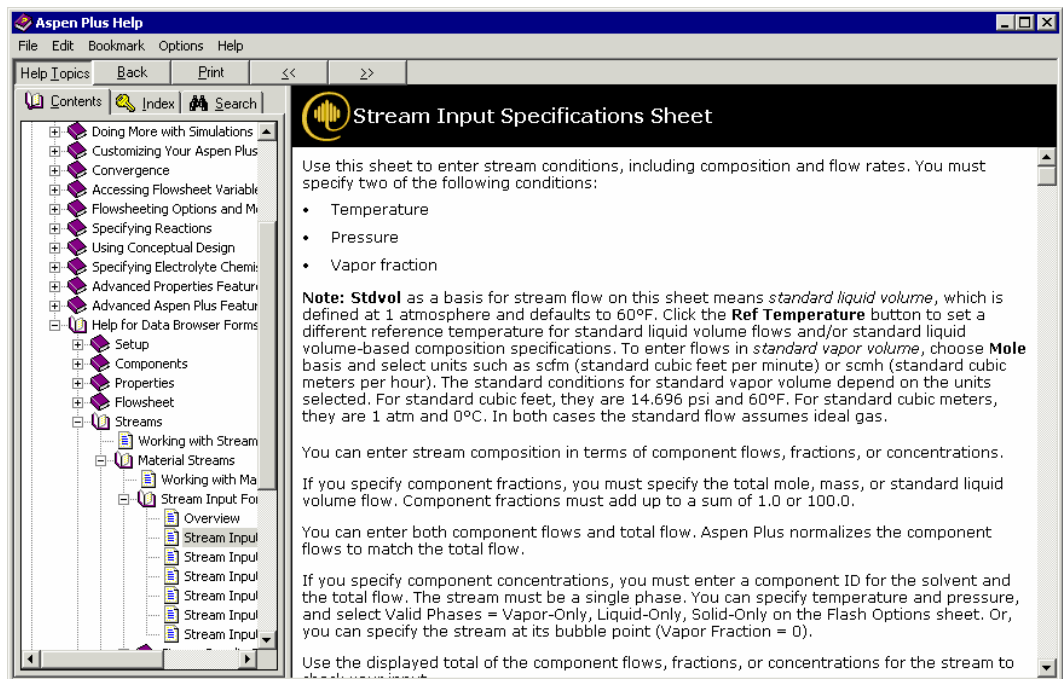
Before specifying the characteristics of Stream 1 you may wish to get context-sensitive help about the sheet itself, the form to which it belongs, or about the various fields within the sheet. There are a number of ways to do this:

- Click , then click the box or sheet.
-or-
- From the Aspen Plus menu bar, click **Help**, select **What's This?**, then click the box or sheet.
-or-
- Click the box or sheet, then press **F1** (the help key).


Get help on the **Stream 1 Input Specifications** sheet and on the whole input form.


- 1 Click .
- 2 Click the tab labeled **Specifications**.

Aspen Plus displays a help window that explains how to use the **Stream Input Specifications** sheet:



If you click the [Stream Input Form](#) link at the bottom of this help window, Aspen Plus displays the help for the Stream Input form, which, in this case, consists of five sheets: **Specifications**, **Flash Options**, **PSD**, **Component Attr.**, and **EO Options**.

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




- 3 Scroll to the end of the help topic and click the green underlined text [Stream Input Form](#).
The **Stream Input Form** help topic appears.
- 4 When finished, click  to close the help window.

To Get Help on any Topic

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

- 1 From the Aspen Plus menu bar, select **Help**.
- 2 Use the **Up** and **Down** arrow keys on the keyboard to move through the **Help** menu.
- 3 Read the descriptions for each item at the bottom left corner of the screen.
- 4 From the **Help** menu, select **Help Topics**.
- 5 In the **Contents** pane at the left, double-click **Using Aspen Plus**.

Tip: You can click the **Help Topics** button in 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.

- 6 Double-click a topic labeled with the  icon to display the associated help window or double-click items labeled with the  icon to view more topics.
- 7 When finished, click  to close the help window.

Entering Data on a Sheet

Once an input sheet is open, 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 in the **Stream 1 Input Specifications** sheet to make it active.
- 2 Enter the following state variable and component flow specifications:

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 **Stream 1 Input Specifications** sheet appears below (the Data Browser menu tree is not shown):

Substream name: MIXED

Ref Temperature

State variables

Temperature: 180 F

Pressure: 20 psia

Total flow: Mole lbmol/hr

Solvent:

Composition

Mole-Flow lbmol/hr

Component	Value
METHANOL	50
WATER	50

Total: 100

When all required specifications have been entered, a check mark (✓) appears on the tab containing the sheet name. Check marks also appear in the Data Browser menu tree.


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 Sheet

- 1 From the Data Browser, click .

Note: The  button can also be found in the Data Browser toolbar of the main window.

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

Specifications | Flash Options | Entrainment

Flash specifications


Temperature [] F []

Pressure [] psi []

Valid phases

Vapor-Liquid []



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:

Completion Status

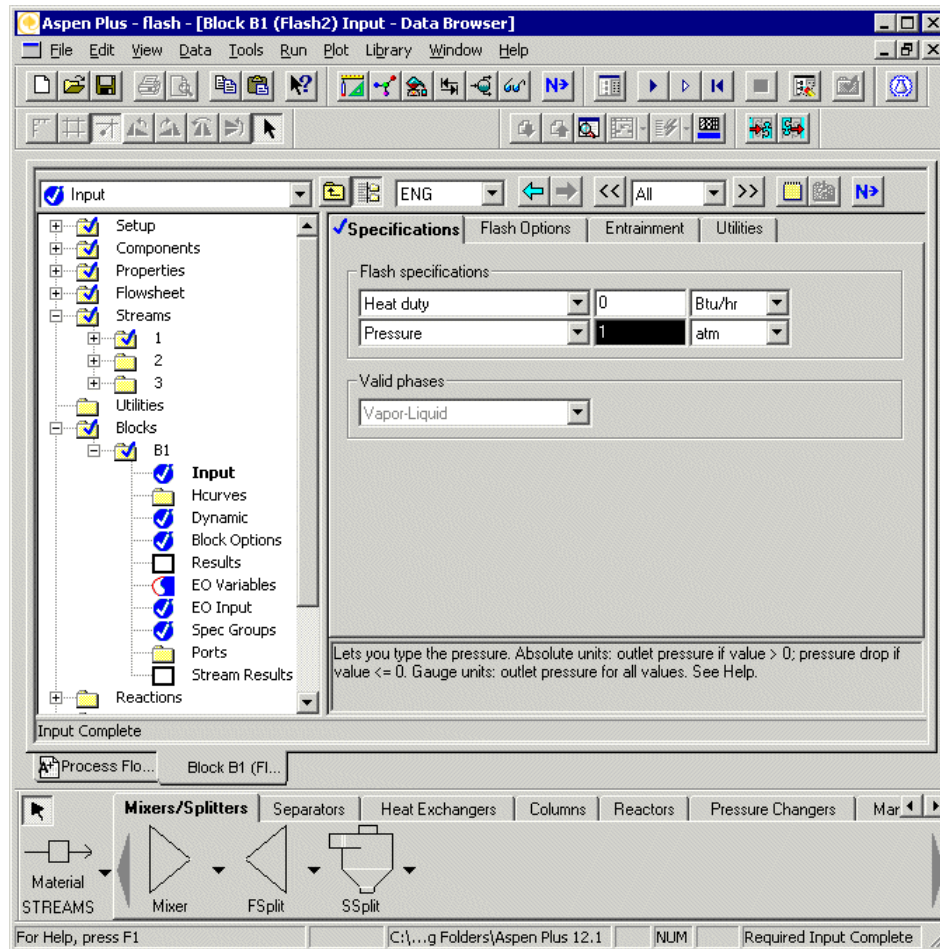
Two of Temperature, Pressure, Vapor Fraction, and Heat Duty (or inlet heat stream without outlet heat stream) must be specified.

Click  to close the **Completion Status** message box.

- 2 Change the first field in the **Flash specifications** area from Temperature to Heat Duty by clicking  and selecting **Heat Duty** from the list.
- 3 In the Heat Duty value field, type **0**. There is no need to change the units (Btu/hr is the default).
- 4 Make sure the first field in the second line of the **Flash specifications** area reads **Pressure**, then type **1** in the Pressure value field.
- 5 In the Pressure units field, click  and select **atm** to change the input units from psia to atm.
- 6 The box in the **Valid phases** area is set to **Vapor-Liquid** by default. For this simulation, accept the default.

Note: Default options on Data Browser sheets appear shaded unless you modify them, in which case they will appear in black text.

The input data on the **Block B1 Input Specifications** sheet is now complete:






The checkmarks in the Data Browser menu tree and the absence of partially filled circles indicates that all required data have been entered. The *Input Complete* message in the lower left corner of the Data Browser window confirms that Block B1 is fully specified and the *Required Input Complete* message in the lower right corner of the main window confirms that all blocks and streams are ready for a simulation run.

Note: The Data Browser window is on top of the process flowsheet window. To look at your process flowsheet, click its tab. Alternatively, click **Windows** from the Aspen Plus menu bar, and select **Process Flowsheet Window**.

Running the Simulation

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

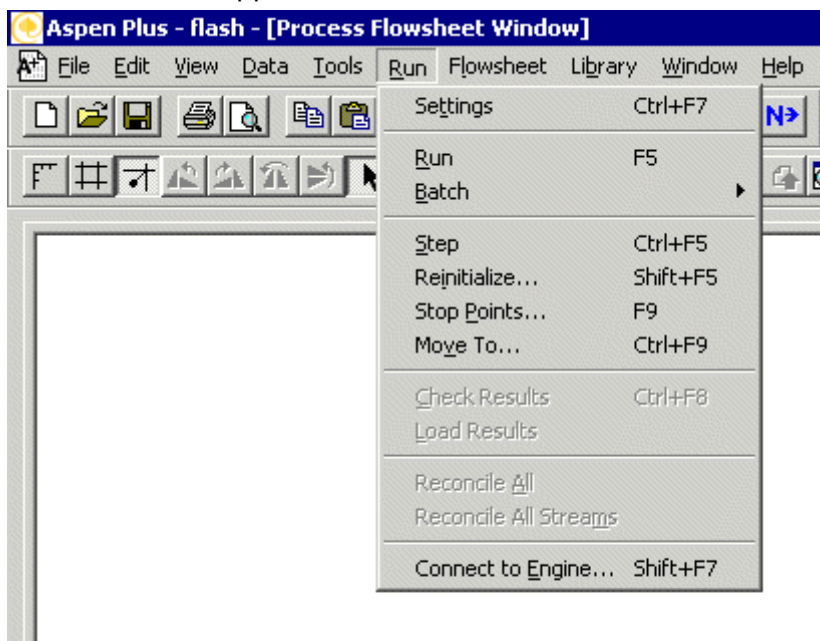
- From the Aspen Plus menu bar, select **Run**, and then select **Run**.
- From the Aspen Plus toolbar, click .
- Click  to open the Control Panel and then click  from the Control Panel.
- Press **F5**.

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

To Run the Simulation

- 1 From the Aspen Plus menu bar, click **Run**.

The **Run** menu appears:



- 2 From the **Run** menu, select **Run**.

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. In the status bar at the bottom of the main window, the prompt message *Simulation run completed* appears on the left, and on the right, the status message *Results Available* appears in blue.

Note: If the calculations are completed with errors or warnings, the status message indicates *Results Available with Errors* and *Results Available with Warnings*, respectively.

Examining Stream and Block Results

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

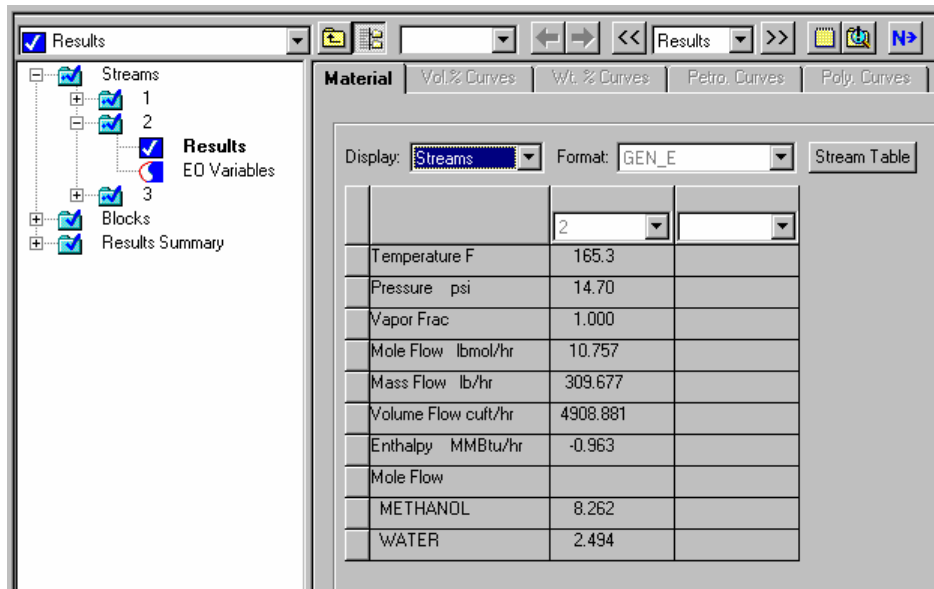
To Display the Flash Overhead Vapor (Stream 2) Results

- 1 Display the process flowsheet by clicking its tab.

Note: If the streams in your process flowsheet now have temperature and pressure data attached to them, you can remove these attachments by clicking **View** and selecting **Global Data**. Or, you may wish to click **View**, select **Zoom**, and then select **Zoom Out** or **Zoom Full** 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 Data Browser window opens with the **Streams | 2 | Results | Material** sheet in view, providing the thermodynamic state and composition flows of the vapor stream:

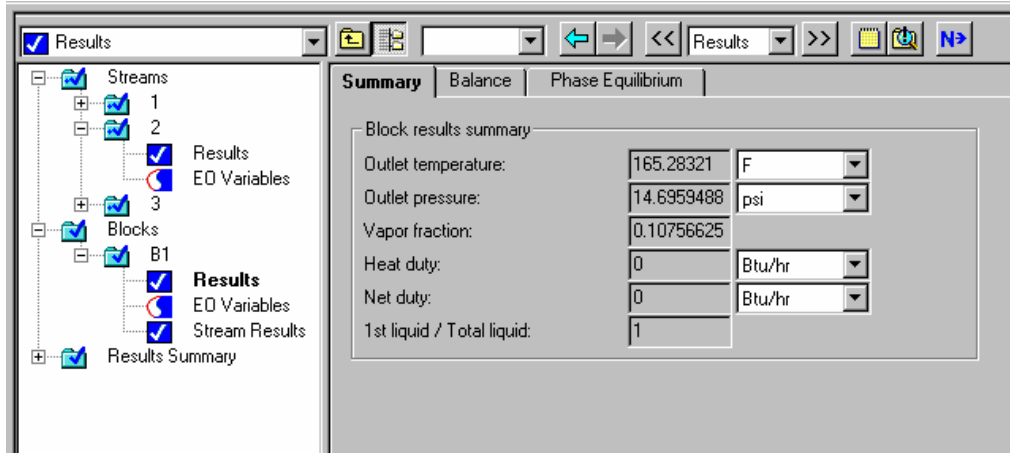



Property	Value	Unit
Temperature	165.3	F
Pressure	14.70	psi
Vapor Frac	1.000	
Mole Flow	10.757	lbmol/hr
Mass Flow	309.677	lb/hr
Volume Flow	4908.881	cuft/hr
Enthalpy	-0.963	MMBtu/hr
Mole Flow		
METHANOL	8.262	
WATER	2.494	


- 4 If necessary, use the vertical scrollbar to view the stream results.
- 5 From the Data Browser menu tree, select **Blocks | B1**.

Note: You can expand menu tree items by clicking the **+** symbol next to a closed folder. When you select a new folder, it automatically expands with the first item selected.

The **Block B1 Results Summary** sheet appears with the overall results for the block:



- 6 Review the calculated flash outlet temperature and overall vapor fraction.
- 7 Click  to browse through the results. Alternatively, click the **Balance** and **Phase Equilibrium** tabs.

Note: Use  to browse through all available sheets according to your position in the Data Browser menu tree.

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 Data Browser window opens with the **Streams | 1 | Input | Specifications** sheet in view.
- 3 In the Composition area, enter the following values for the component mole-flows:

Component	Value
Methanol	60
Water	40

- 4 From the Aspen Plus menu bar, click **Run**, then select **Run** 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

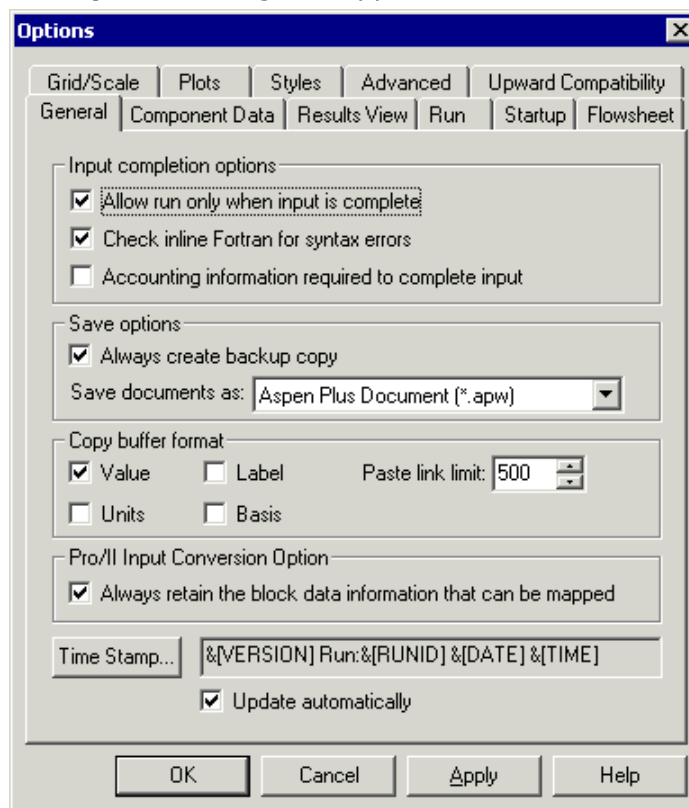
For this example, save your file as both an Aspen Plus document (.apw) file and an Aspen Plus backup (.bkp) file. Document files contain all the intermediate convergence information from the simulation and are useful for saving long simulations. Document files are *not* forward compatible for new versions of Aspen Plus.

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 From the Aspen Plus menu bar, select **Tools** and then select **Options**. The **Options** dialog box appears:

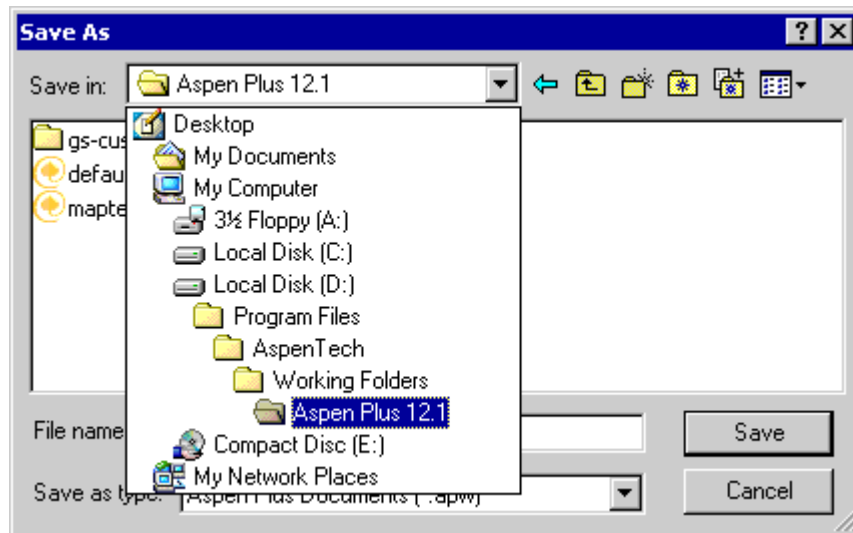


- 2 On the **General** tab, in the Save options area, select the checkbox next to **Always create backup copy**, if it is not already checked.
- 3 Make sure **Aspen Plus documents (*.apw)** appears in the **Save documents as** field.
- 4 Click **OK**.

Next, save the simulation and exit Aspen Plus.

To Save and Exit

- 1 From the Aspen Plus menu bar, select **File** and then select **Save As**. The **Save As** dialog box appears:



- 2 If necessary, use the **Save in** list to navigate to your Aspen Plus working folder. In this example, the folder is located in D:\Program Files\AspenTech\Working Folders\Aspen Plus <version>.
- 3 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 From the Aspen Plus menu bar, 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

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 Build a process flowsheet.

Defining the Simulation: Methylcyclohexane Recovery Column

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

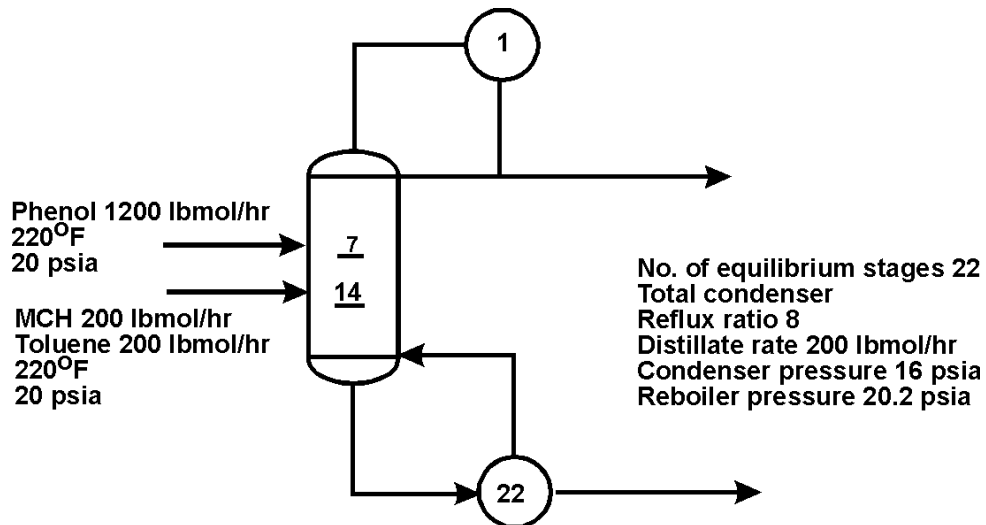


Figure 2.1 Simulation Definition: MCH Recovery Column

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 methylcyclohexane 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 **Aspen Engineering Suite**, then **Aspen Plus <version>**, then **Aspen Plus User Interface**.

The **Aspen Plus Startup** dialog box appears. Create a new simulation using an Aspen Plus built-in template.

Creating a New Simulation

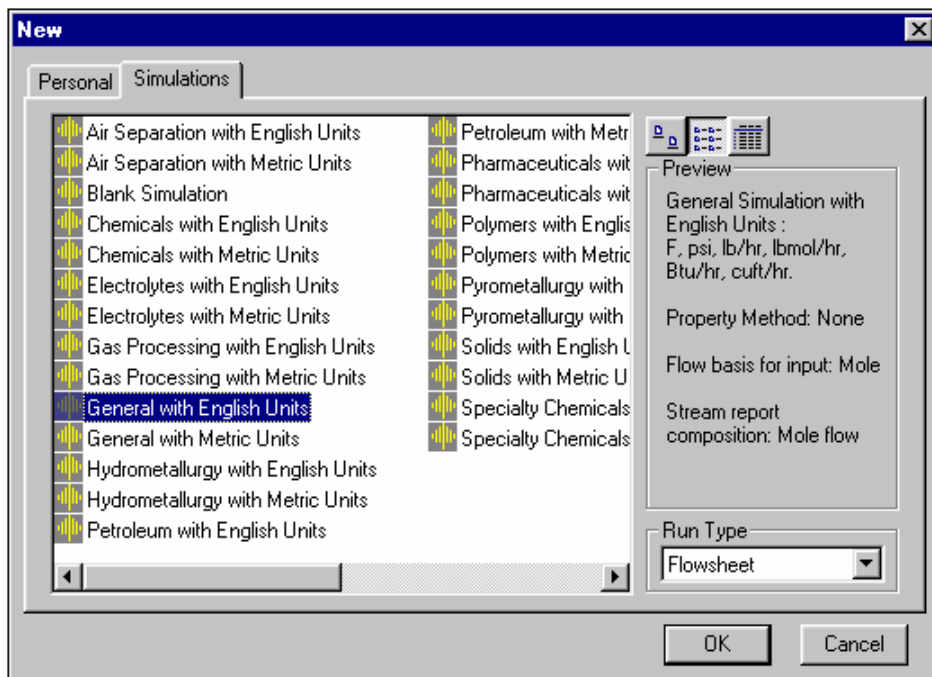
Aspen Plus provides built-in templates for applications such as chemicals, petroleum, electrolytes, specialty chemicals, pharmaceuticals, and metallurgy.

- 1 In the **Aspen Plus Startup** dialog box, select **Template** and click **OK**.
The **New** dialog box appears.

Note: Use the **New** dialog box to specify the Application Type and the Run Type for the new run. Aspen Plus uses the Application Type you choose to automatically set various defaults appropriate to your application.

To Specify the Application Type and Run Type for the New Run

- 2 Select the **General with English Units** template.
The default Run Type, **Flowsheet**, is appropriate for this simulation.



- 3 Click **OK** to apply these options.

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

Note: If the **Connect to Engine** dialog box appears, see "[Connecting to the Aspen Plus Simulation Engine](#)" on page 93.

The Aspen Plus main window is now active.

The Aspen Plus Main Window


The main window appears when you start Aspen Plus. Because you have not entered any simulation specifications yet, the workspace is blank.

For more information about this window, see "[The Aspen Plus Main Window](#)" on page 7.


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.

Note: If you click  before building the process flowsheet, Aspen Plus displays the **Flowsheet Definition** dialog box, informing you that the first step is to build the process flowsheet. Click **OK** and build the flowsheet.

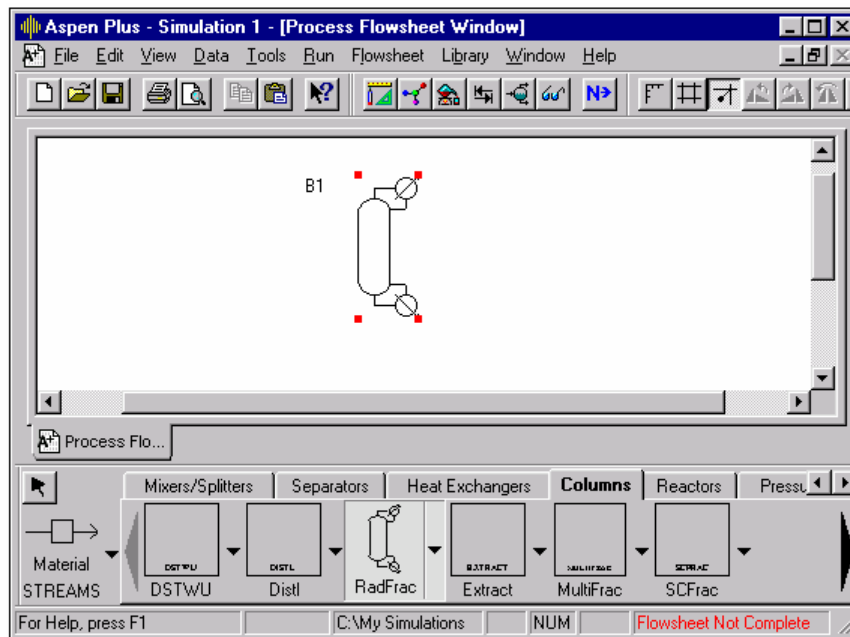
To Select a Unit Operation Block

- 1 From the Model Library at the bottom of the Aspen Plus Process Flowsheet Window, select 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 in the lower left of the window.
- 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 Click  at the top of the Help window to close it.
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 Select the icon labeled **FRACT1** and drag it (click and hold) into your process flowsheet. This will allow you to place a single block onto your process flowsheet.
- 4 Move the mouse to the middle of the workspace and release the mouse button.

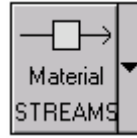
The block appears on the flowsheet with the default name **B1**:

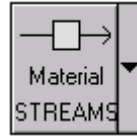



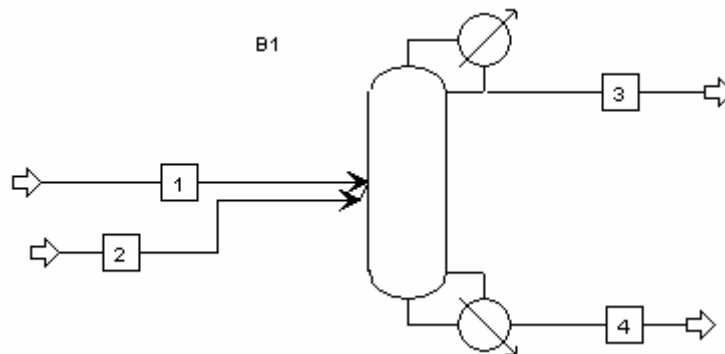
Notes about block placement:

- **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  when finished.
- To stop the automatic naming of blocks, select **Tools**, then **Options**, then the **Flowsheet** tab and then clear the appropriate checkbox.
- Your RadFrac block may have a 3-D appearance. The **3D icon** option on the **Tools | Options | Styles** tab determines whether these icons are used.

To Connect Streams to the Block



- 1 From the Model Library, 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 (named Stream 1 by default) at that location.
- 5 Create another material feed stream (named Stream 2 automatically) 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 right 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 button and choose either the Heat or Work stream icon.
- To cancel connecting a stream at any time, press the Escape key.
- 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 select **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 in the **Model Library** and drag to place a single stream. Drag to a port and release the 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 **Data Browser** input sheets to enter the remaining required information for this run.

The Aspen Plus **Next** function displays the required input sheets automatically. You can also navigate to an input sheet in any of the following ways:

- Click **Data** in the Aspen Plus menu bar and select the sheet you want.
- Click **Data** on the Aspen Plus menu bar, select **Data Browser**, and use the menu tree to navigate to any input sheet.
- Click the button that corresponds to the sheet you want from the Data Browser toolbar:

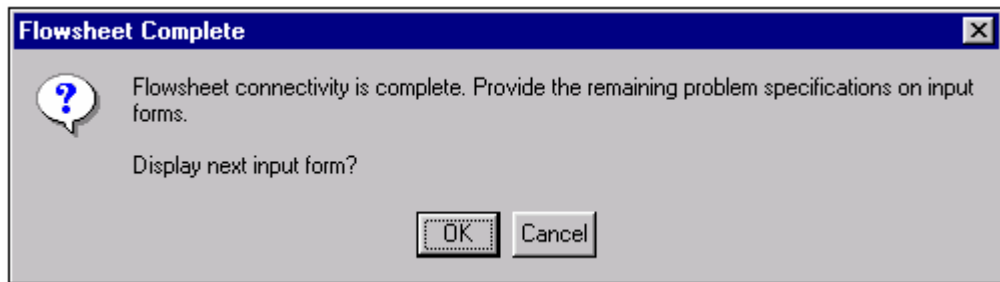


- Select a stream or block in the process flowsheet, right-click, and then select **Input** on the shortcut menu.
- Double-click a stream or block in the process flowsheet.

Specifying a Title for the Simulation

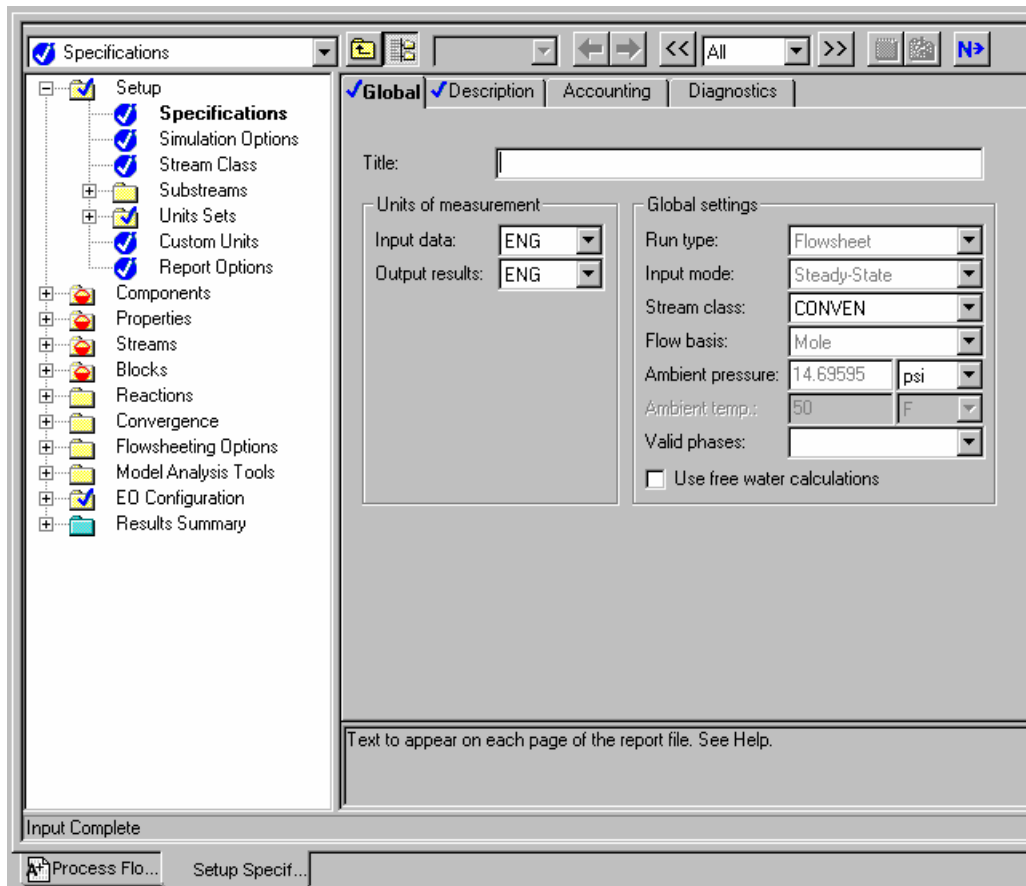
- 1 Click .

Aspen Plus displays the **Flowsheet Complete** dialog box indicating that your flowsheet is complete and that you need to provide remaining specifications.



- 2 Click **OK** to display the first required input sheet.

Aspen Plus opens the Data Browser window containing the Data Browser menu tree and the **Setup | Specifications | Global** sheet:



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

The **Setup | Specifications | Global** sheet 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 the **Setup | Report Options** form by clicking once on the **Report Options** form under the **Setup** folder in the Data Browser menu tree.

Note: If the **Report Options** form is not visible click the \oplus 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.

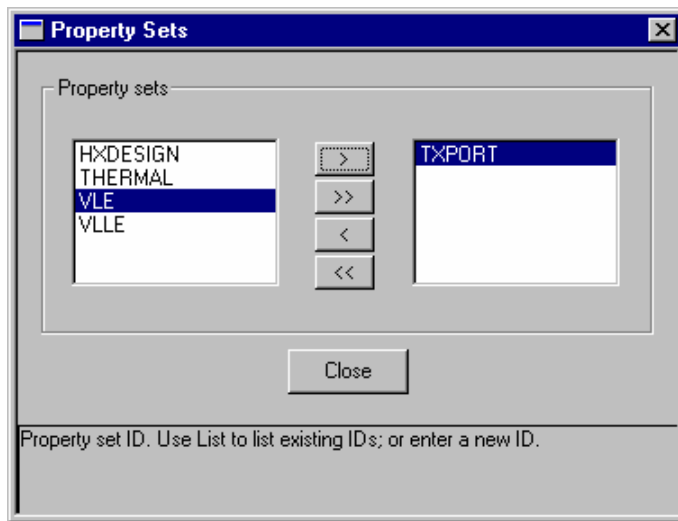
- 2 Click the **Stream** tab.
- 3 In the **Fraction basis** area, select the **Mole** checkbox.

The screenshot shows the 'Report Options' dialog box with the 'Stream' tab selected. The 'Items to be included in stream report' section is expanded, showing two columns: 'Flow basis' and 'Fraction basis'. In the 'Fraction basis' column, the 'Mole' checkbox is checked and circled. Other options include 'Generate a standard stream report', 'Include stream descriptions', 'Stream format' (set to GEN_E), and 'Sort streams alphanumerically'. Buttons for 'Include Streams', 'Exclude Streams', 'Property Sets', and 'Component Attributes' are visible at the bottom.


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 | Creating a Simulation Model** and **Using Aspen Plus | Advanced Properties Features | Property Sets**.

- 6 Click **Close**.
- 7 Click .
- The Components | Specifications | Selection sheet appears.

Entering Components

Use the **Components | Specifications | Selection** sheet to select the chemical components present in the simulation.

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 **Formula** fields automatically.
- 2 In the next **Component ID** field, type PHENOL and press **Enter** on the keyboard.
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 row, type METHYLCYC in the **Component name** field and press **Enter** on the keyboard.

The **Find** dialog box appears, listing all the components in the Aspen Plus databank that have a name containing METHYLCYC:

Component name	Formula	Alternate name	Databank	MW
METHYLCYCLOPE...	C8H12-2	CYCLOPENTANE, ...	PURE12	84.1613
1,1-DIMETHYLCYC...	C7H14-2	CYCLOPENTANE, ...	PURE12	98.1882
CIS-1,2-DIMETHYL...	C7H14-3	CYCLOPENTANE, ...	PURE12	98.1882
TRANS-1,2-DIMET...	C7H14-4	CYCLOPENTANE, ...	PURE12	98.1882
CIS-1,3-DIMETHYL...	C7H14-E2	CYCLOPENTANE, ...	PURE12	98.1882
TRANS-1,3-DIMET...	C7H14-E3	CYCLOPENTANE, ...	PURE12	98.1882
1-METHYL-1-ETHY...	C8H16-13	1-ETHYL-1-METH...	PURE12	112.215
METHYLCYCLOHE...	C7H14-6	CYCLOHEXANE, ...	PURE12	98.1882
1,1-DIMETHYLCYC...	C8H16-1	CYCLOHEXANE, 1...	PURE12	112.215

- 5 From the list, locate and select **Methylcyclohexane**.

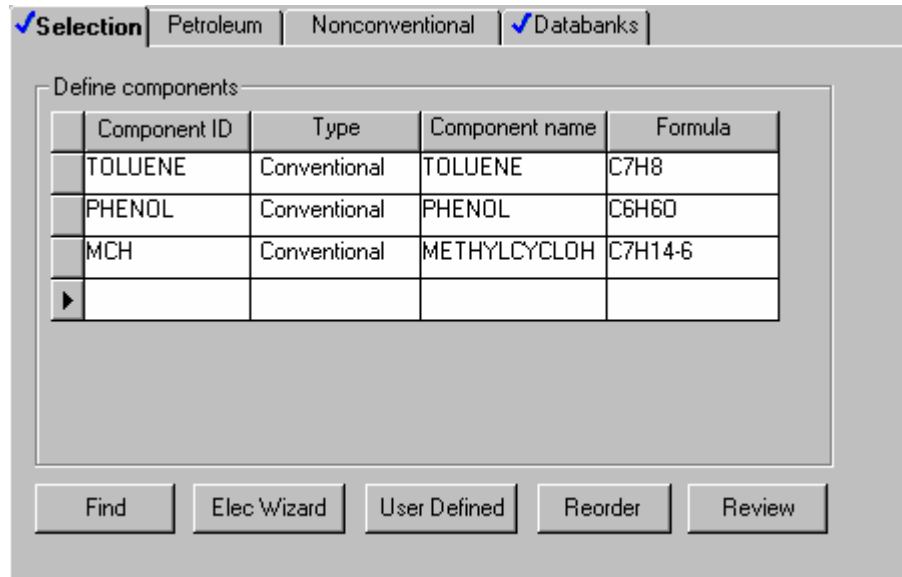
Note: To view the complete component names, click and drag the right edge of the **Component name** column to the right.

- 6 Click **Add**.

- 7 Click **Close**.

Note: If you need to search for components based on molecular weight range, boiling point range, or CAS numbers, use the **Advanced** sheet in the **Find** dialog box.

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



8 Click .

The **Properties | Specifications | Global** sheet appears.

Selecting Thermodynamic Methods

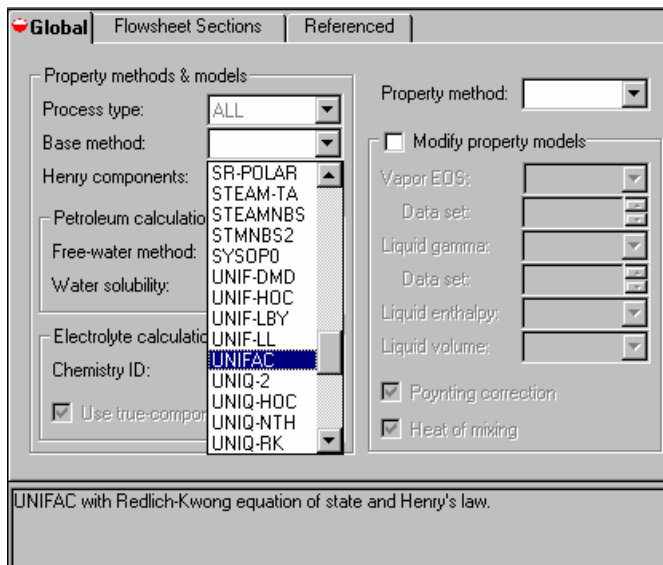
Use the **Properties | Specifications | Global** sheet to select the property method used to calculate properties such as K-values, enthalpy, and density. The **Base method** list contains various property methods built into Aspen Plus. The specific methods in the list depend on the chosen **Process type**. To see all the available methods (a very long list), choose Process type **ALL**.

Note: Clicking the **Modify property models** checkbox 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 Data for Simulations | 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

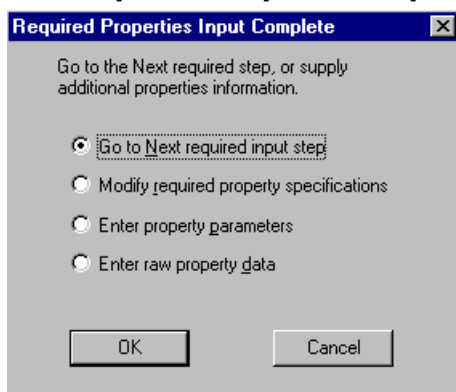
- 1 In the **Base method** list, click  to display the available property methods in Aspen Plus:




Get a brief description of a base method by selecting it and reading the prompt. For detailed information about a base method, highlight the name and use the **What's this?** help utility or refer to the *Physical Property Methods and Models* reference manual.

- 2 From the **Base method** list, use the vertical scrollbar and select **UNIFAC**.
- 3 Click .

The **Required Properties Input Complete** dialog box appears:



- 4 Click **OK**.
Aspen Plus displays the next sheet that requires input.

Note: You can navigate to the incomplete sheets yourself by clicking on folders in the menu tree marked with the  symbol.

Entering Stream Data

The **Streams | 1 | Input | Specifications** sheet appears next. Make Stream 1 the MCH-Toluene feed stream.

- 1 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 **Streams | 1 | Input | Specifications** sheet is complete:

Substream name: MIXED

Ref Temperature

State variables:

Temperature: 220 F

Pressure: 20 psia

Total flow: Mole lbmol/hr

Solvent:

Composition:

Mole-Flow: lbmol/hr

Component	Value
TOLUENE	200
PHENOL	
MCH	200

Total: 400

- 2 Click .

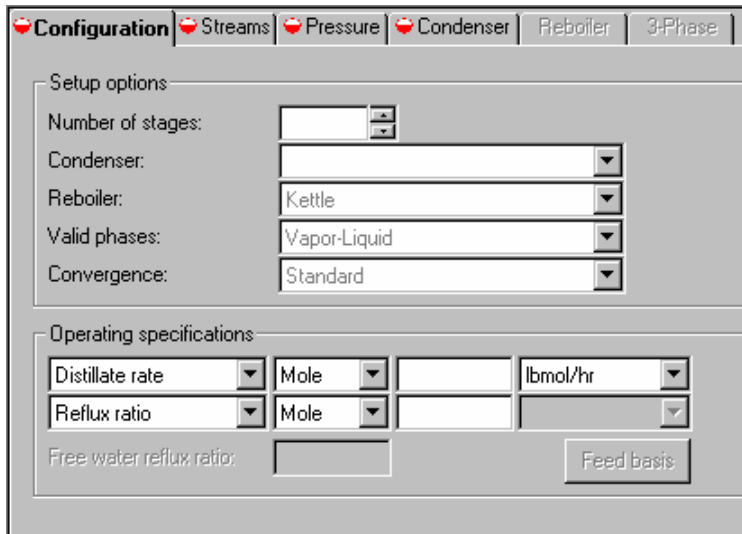
The **Streams | 2 | Input | Specifications** sheet appears. Make Stream 2 the phenol feed stream.

- 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 **Blocks | B1 | Setup | Configuration** sheet appears:

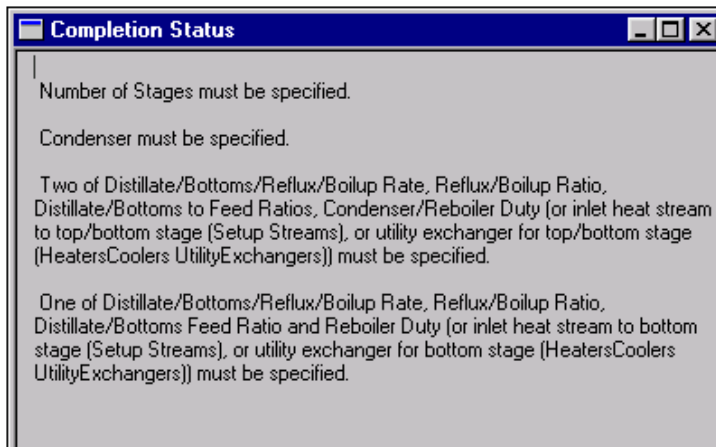


Entering Unit Operation Block Data

On the **Blocks | B1 | Setup | Configuration** sheet, 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 prompts at the bottom of the sheet.

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



Click  to 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 checkmark on the **Configuration** tab indicates the sheet is complete:

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

The **Blocks | B1 | 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 3.1, 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 **Blocks | B1 | Setup | Streams** sheet is complete:

Feed streams			
	Name	Stage	Convention
▶	1	14	Above-Stage
	2	7	Above-Stage

Product streams								
	Name	Stage	Phase	Basis	Flow	Units	Flow ratio	Feed specs
	3	1	Liquid	Mole		lbmol/hr		Feed basis
	4	22	Liquid	Mole		lbmol/hr		Feed basis

7 Click

The **Blocks | B1 | 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**.

13 Accept the default Pressure units (psia).

The completed **Block B1 Setup Pressure** sheet looks like this:

View:

Pressure profile	
Stage	Pressure
	psia
1	16
22	20.2
*	

14 Click

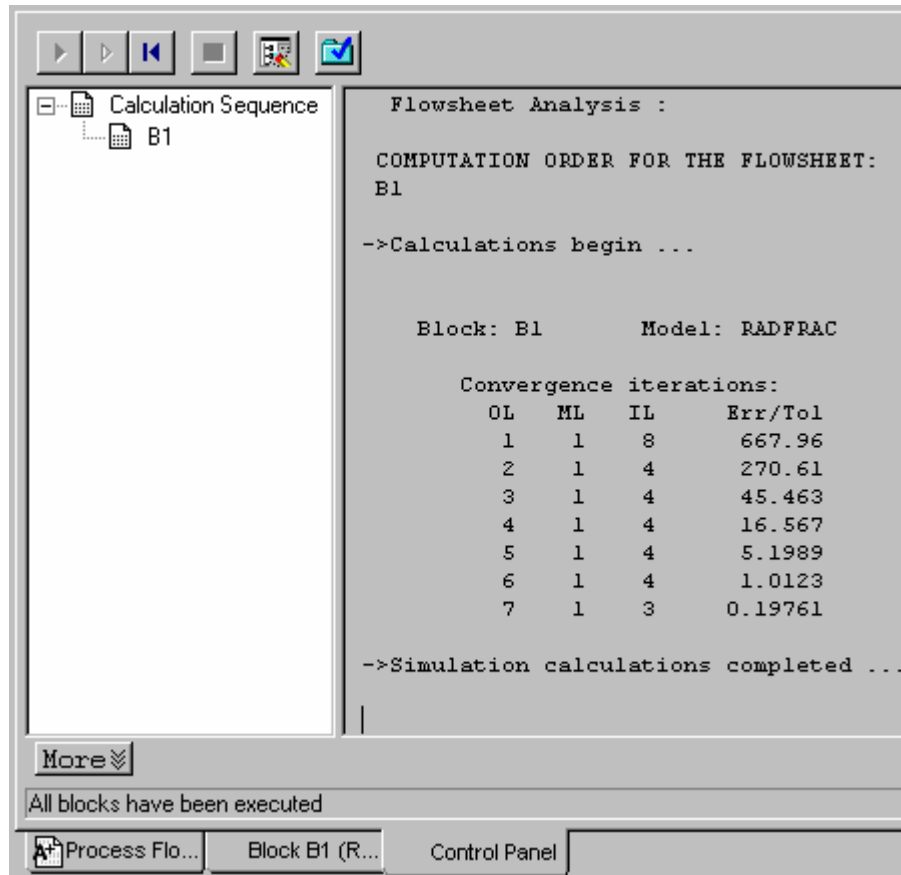
The **Required Input Complete** dialog box appears.

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 dialog box and scroll through the Data Browser 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 *All blocks have been executed* appears in the status bar.

Note: There are 3 tabs at the bottom of the active form that can be used to navigate between the overlapping windows. For example, to view the

Process Flowsheet Window, click the  tab. If you don't see the tabs, from the **Window** menu select **Workbook**.

Examining Simulation Results

When the simulation completes, the *Results Available* message appears in the status bar at the bottom of the main window. Now you can examine the results of your simulation.

- 1 Navigate to the process flowsheet in one of these ways:
 - o Click the **Process Flowsheet** tab, or
 - o Select **Window | Process Flowsheet Window** from the Aspen Plus menu bar.

To Display the Results for Block B1

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

Note: Your flowsheet may now have some pressure and temperature data displayed. You can turn this feature on and off by selecting **View | Global Data**. You may also wish to alter the appearance of your flowsheet by selecting, for example, **View | Zoom | Zoom Full**.

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

The **Block B1 Results Summary** sheet appears:

Condenser / Top stage performance		
Temperature:	218.828654	F
Heat duty:	-24173465	Btu/hr
Subcooled duty:		
Distillate rate:	200	lbmol/hr
Reflux rate:	1600	lbmol/hr
Reflux ratio:	8	
Free water distillate rate:		
Free water reflux ratio:		



For this run, block results are reported on three forms: **Results Summary**, **Profiles**, and **Stream Results**. In the Data Browser menu tree, a checkmark in a square appears next to each form to indicate that they contain results.

- 4 From the Data Browser menu tree, select **Blocks | B1 | Profiles** by clicking once on **Profiles**.

The **Block B1 Profiles TPFQ** sheet appears, reporting temperature, pressure, heat duty, and flow profiles for the block:

The screenshot shows the 'TPFQ' window with the 'Profiles' tab selected. The 'View' is set to 'Summary' and the 'Basis' is 'Mole'. The table displays the following data:

Stage	Temperature	Pressure	Heat duty	Liquid flow	Vapor flow
	F	psi	Btu/hr	lbmol/hr	lbmol/hr
1	218.828654	16	-24173465	1600	0
2	219.689481	16.2	0	1599.83084	1800
3	220.589774	16.4	0	1598.4381	1799.83084
4	221.584878	16.6	0	1594.18633	1798.4381
5	222.835118	16.8	0	1580.59799	1794.18633
6	225.036821	17	0	1504.5433	1780.59799
7	235.916902	17.2	0	2891.99498	1704.5433
8	236.867831	17.4	0	2894.04179	1891.99498
9	237.883187	17.6	0	2895.1759	1894.04179
10	239.002376	17.8	0	2895.08779	1895.1759
11	240.285834	18	0	2893.54583	1895.08779

- 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 Data Browser menu tree, the  button, and/or the tabs on each form to view the rest of the results for Block **B1**.
- 10 Check the purity of the methylcyclohexane overhead product by examining the composition at the top of the column (stage 1).

The screenshot shows the 'TPFQ' window with the 'Compositions' tab selected. The 'View' is set to 'Vapor' and the 'Basis' is 'Mole'. The table displays the following data:

Stage	TOLUENE	PHENOL	MCH
1	0.02610161	0.00062651	0.97327187
2	0.02609472	0.00131022	0.97259505
3	0.02609067	0.00259752	0.9713118
4	0.02610349	0.00508974	0.96880675
5	0.02615863	0.01020908	0.96363228
6	0.02630456	0.02216903	0.9515264
7	0.02660271	0.06053092	0.91286636

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 **Stream Results Material** sheet appears, providing the results for Stream 3:

Stream	Property	Value
3	Temperature F	218.8
3	Pressure psi	16.00
3	Vapor Frac	0.000
3	Mole Flow lbmol/hr	200.000
3	Mass Flow lb/hr	19605.002
3	Volume Flow cuft/hr	449.995
3	Enthalpy MMBtu/hr	-14.509
3	Mole Flow lbmol/hr	
3	TOLUENE	5.219
3	PHENOL	0.262
3	MCH	194.519
3	Mole Frac	


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 checkbox in the **Setup | Report Options | Stream** sheet.

To Display the Results for All Streams on the Same Sheet

- 1 In the **Stream Results Material** sheet, click the list 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** list box.

Note: You can close or minimize some of the overlapping windows if you wish. Click the tab for a window and then use the lower row of control buttons





in the upper right corner of the screen: .


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 **Process Flowsheet** window.
- 2 Select Stream 2, and right-click to display the shortcut menu.
- 3 Select **Input**.
The **Stream 2 Input Specifications** sheet appears.
- 4 In the **Composition** area, 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, *Input Changed* messages appear in the prompt areas of the main window and in the Data Browser window. Also, the symbols  and  appear in several places in the Data

Browser menu tree. Finally, the run button  and the **Run | Run** menu command are 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 Control Panel appears and 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 Data Browser.


Note: You can display the complete Data Browser menu tree by clicking the  button, or by selecting **Data | Data Browser** from the Aspen Plus menu bar, or by pressing **F8**.

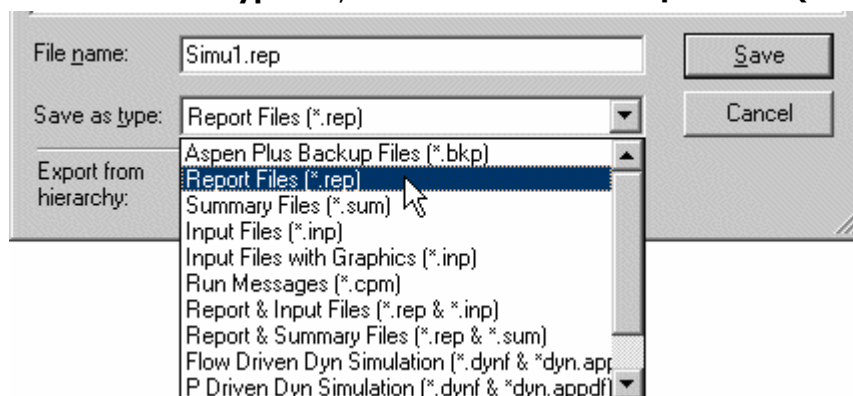
MCH purity with the increased phenol flow rate is now over 98%. To choose an optimal flow rate, it would be helpful to generate a plot of MCH purity versus phenol flow rate. This is the subject of Chapter 3: *Performing a Sensitivity Analysis*.

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 Aspen Plus menu bar, select **File** and then select **Export**.
The **Export** dialog box appears.
- 2 In the **Save as type** list, click  and select **Report File (*.rep)**.



- 3 In the **File name** list, 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** list). 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 selecting **View | Report** from the Aspen Plus menu bar. 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 thing, 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 Aspen Plus menu bar, select **File | Save as**.
- 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 | Aspen Engineering Suite | Aspen Plus <version> | Aspen Plus User Interface**.

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

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 In the **Aspen Plus Startup** dialog box, make sure **Open an Existing Simulation** is selected.
- 2 In the list, select **MCH.apw** and click **OK**.

-or-

If Your Saved File MCH.apw is not Displayed

- 1 In the **Aspen Plus Startup** dialog box, make sure **Open an Existing Simulation** is selected.
- 2 In the list box, double-click **More Files**, or click **OK** without selecting anything in the list box.
The **Open** dialog box appears.
- 3 Navigate to the directory containing your saved **MCH.apw** or navigate to the **Examples** 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.

- 4 Select either **MCH.apw** or **MCH.bkp** and click **Open**.

Note: If the **Connect to Engine** dialog box appears, see "[Connecting to the Aspen Plus Simulation Engine](#)" on page 93.

The **Process Flowsheet** window for 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 Aspen Plus menu, select **File** and then **Save As**.
- 2 In the **Save As** dialog box, choose the directory where you want to save the simulation.
- 3 In the **File name** field, enter **MCHSENS**.
- 4 In the **Save as type** field, make sure **Aspen Plus Documents (*.apw)** is selected.
- 5 Click **Save**.

Defining the Sensitivity Analysis

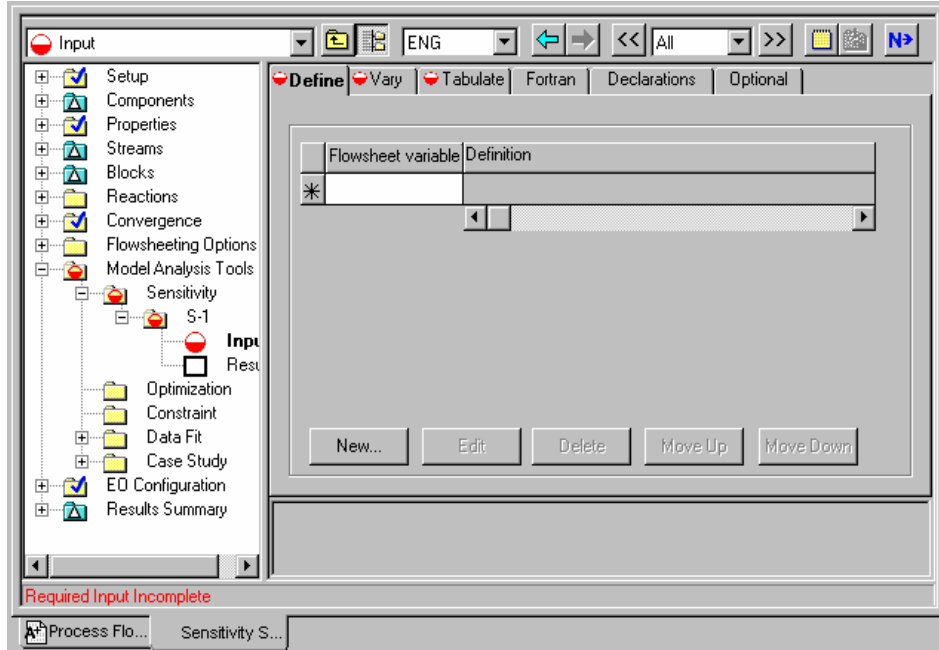
In Chapter 2, you simulated MCH recovery using two values for the phenol solvent flow rate. In the following sensitivity analysis, tabulate methylcyclohexane (MCH) distillate product purity (mole fraction), as well as condenser duty and reboiler duty, for several different flow rates of phenol.

Entering Sensitivity Specifications

To Create a New Sensitivity Block

- 1 Select **Data | Model Analysis Tools | Sensitivity**.
The **Model Analysis Tools | Sensitivity** object manager appears. You can use this sheet to:
 - o Create new sensitivity blocks.
 - o Edit existing sensitivity blocks.
 - o 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 **Model Analysis Tools | Sensitivity | S-1 | Input | Define** 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.

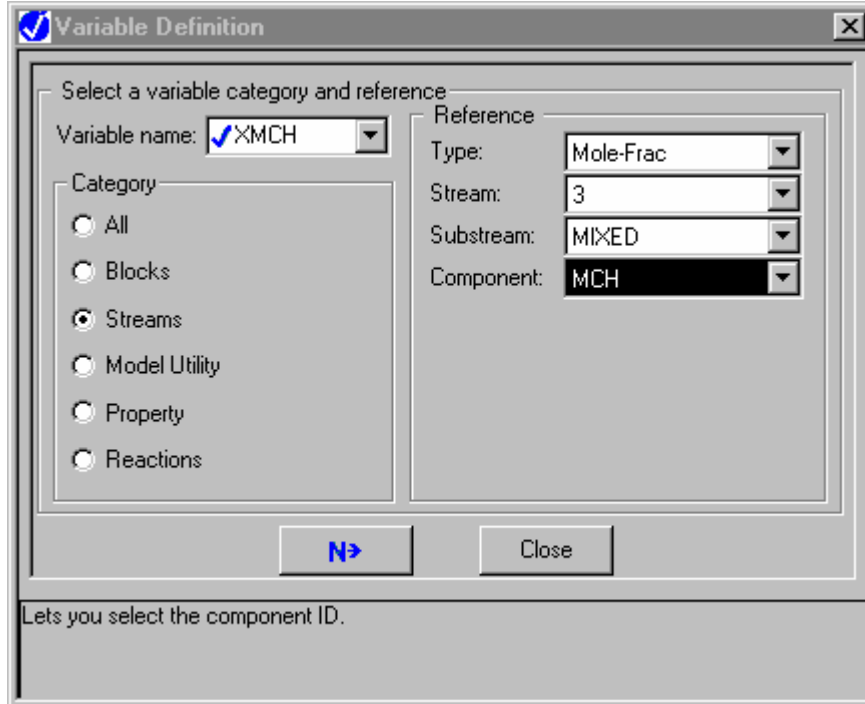
In the **Define** sheet, define names for each of the calculated variables (product purity, condenser duty, reboiler duty). In the **Vary** sheet, specify the range and increments for the manipulated variable (phenol flow rate). In the **Tabulate** sheet, set up the format you want for the data table.

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

To Define XMCH as Distillate Product Purity

- 1 On the **Define** sheet, click **New**.
The **Create new variable** dialog box appears.
- 2 Type XMCH and click **OK**.
The **Variable Definition** dialog box appears. 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**.
As you complete the specifications in this dialog box, more fields necessary to complete the variable definition will appear.
- 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.



7 Click **Close**.

The **Model Analysis Tools | Sensitivity S-1 | Input | Define** sheet reappears with the first defined variable, XMCH, listed.

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**.

The **Variable Definition** dialog box appears. Define QCOND to be the condenser duty for the RadFrac Block B1.


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

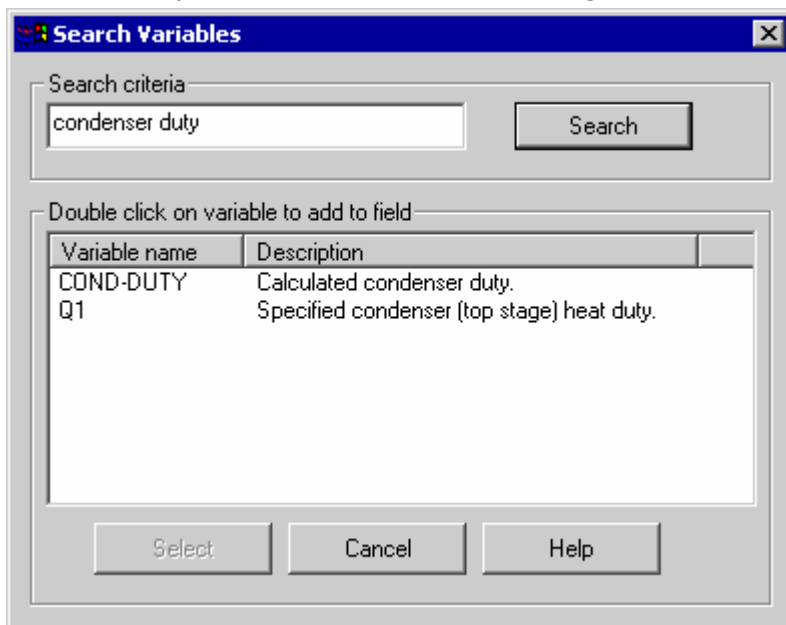
4 In the **Type** field, select **Block-Var**.

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

6 In the **Variable** field, click the drop down button 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.

- 7 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.
- 8 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:



9. 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 **Variable** field and the **Sentence** 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 in the Menu bar, the heat duties would be accessed in Watts.

Do *not* close the dialog box. Instead, define the next variable, QREB.

- 9 In the **Variable name** field, select **<New>**.

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

The **New Item** dialog box appears.

- 10 Type QREB and click **OK**.
Define QREB to be the reboiler duty for Block B1.
- 11 In the **Category** area, select **Blocks**.
- 12 In the **Type** field, select **Block-Var**.
- 13 In the **Block** field, select **B1**.
- 14 Click  next to the **Variable** list, and search for **Reboiler Duty**.

15 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.


16 Click **Close**.

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

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

Next, specify the range, increment size, and label for the phenol flow rate manipulated variable.

To Specify the Manipulated Variable

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


The **Model Analysis Tools | Sensitivity | S-1 | Input | Vary** sheet appears.

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

2 In the **Variable number** field, select **1**.

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

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

Like the Define sheet, the Vary sheet has a search button to help you select the correct variable. 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.

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

6 In the **Values for varied variable** area, select **Overall range** and enter the following values:

Field	Value
Lower	1200
Upper	2000
Incr	100


7 In the **Report labels** area, 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, 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 **Model Analysis Tools | Sensitivity | S-1 | Input | Tabulate** sheet appears. You must identify the variables that you want to appear in the Sensitivity table.
- 2 Press the Fill Variables button to have Aspen Plus tabulate all of the Defined variables automatically.

The completed sheet looks like this:

Column No.	Tabulated variable or expression
1	XMCH
2	QCOND
3	QREB
*	

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.

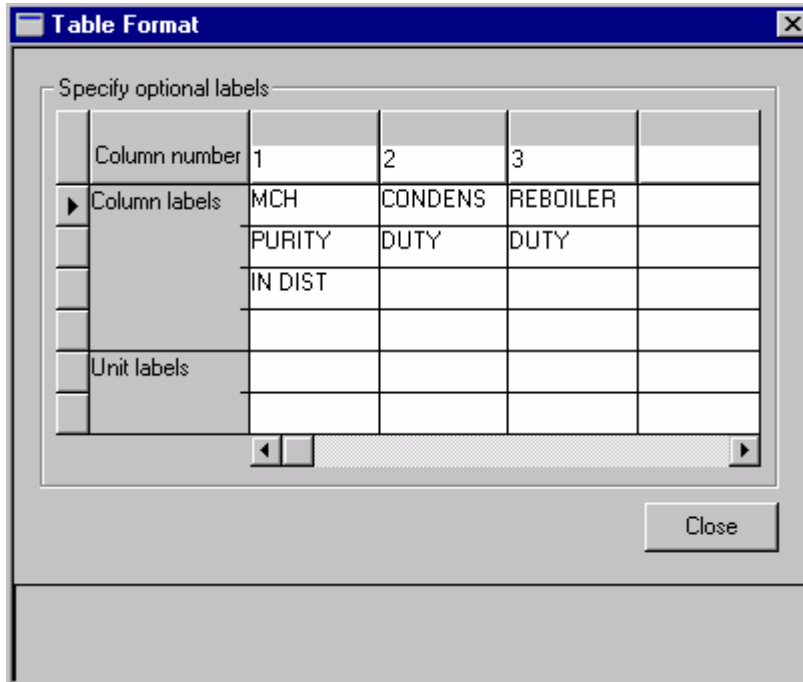
Labels are split into 4 lines for the report file. Each line can contain up to 8 characters.

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 **Model Analysis Tools | Sensitivity | S-1 | Input** 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 Aspen Plus menu bar, select **Run**, and then select **Run**.
- From the Aspen Plus toolbar, click .
- Click  to open the Control Panel and then click  from the Control Panel.
- 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 **Input | Tabulate** sheet, shown as a function of the manipulated variable defined on the **Input | Vary** sheet.

- 1 From the Data Browser menu tree, click **Model Analysis Tools | Sensitivity | S-1 | Results**.

The **Model Analysis Tools Sensitivity S-1 Results Summary** sheet appears:


Summary		Define Variable			
Status	VARY 1 PHENOL FLOWRATE	MCH PURITY IN DIST	CONDENS DUTY	REBOILER DUTY	
	LBMOL/HR		BTU/HR	BTU/HR	
▶ OK	1200	0.97257198	-24173490	31615182.6	
OK	1300	0.9753479	-24170298	32358048.9	
OK	1400	0.97769849	-24167603	33109660	
OK	1500	0.97970757	-24165327	33868528.1	
OK	1600	0.98143328	-24163375	34633649.4	
OK	1700	0.98292353	-24161705	35404199.9	
OK	1800	0.98421708	-24160271	36179496.6	
OK	1900	0.98534612	-24159026	36958966.2	
OK	2000	0.98633569	-24157960	37742126.8	

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.

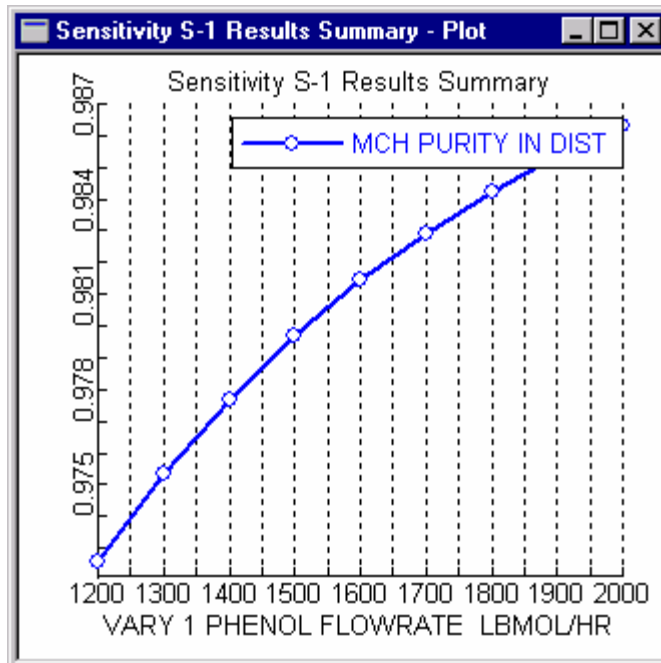
Plotting Sensitivity Results

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

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

- 1 Select the VARY 1 PHENOL FLOWRATE column by clicking its label.
- 2 From the **Plot** menu, select **X-Axis Variable**.
- 3 Select the MCH PURITY IN DIST column by clicking its label.
- 4 From the **Plot** menu, select **Y-Axis Variable**.
- 5 From the **Plot** menu, select **Display Plot**.
A new window with its own tab appears containing the plot you specified.
- 6 Click  in the lower set of control buttons in the upper right corner to reduce the size of the plot and give it a separate window.

The reduced-sized plot looks like this:



- 7 If you wish, customize the plot by clicking the right mouse button in the **Plot** window to access the plot menu.

Saving Your File and Exiting Aspen Plus

- 1 From the Aspen Plus menu bar, select **File | Save as**.
- 2 In the **File name** field, type MCHSENS. 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.

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 | Aspen Engineering Suite | Aspen Plus <version> | Aspen Plus User Interface**.

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

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 In the **Aspen Plus Startup** dialog box, make sure **Open an Existing Simulation** is selected
- 2 In the list, select **MCHSENS.apw** and click **OK**.

-or-

If Your Saved File MCHSENS.apw is Not Displayed

- 1 In the **Aspen Plus Startup** dialog box, make sure **Open an Existing Simulation** is selected
- 2 In the list box, double-click **More Files**, or click **OK** without selecting anything in the list box.

The **Open** dialog box appears.

- 3 Navigate to the directory containing your saved **MCHSENS.apw** or navigate to the **Examples** 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.

- 4 Select either **MCHSENS.apw** or **MCHSENS.bkp** and click **Open**.

Note: If the **Connect to Engine** dialog box appears, see Chapter 8.

The **Process Flowsheet** window for the MCH column simulation appears.

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 **Aspen Plus** menu, select **File | Save As**.
- 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 In the **Save as type** field, make sure **Aspen Plus Documents (*.apw)** is selected.
- 5 Click **Save**.

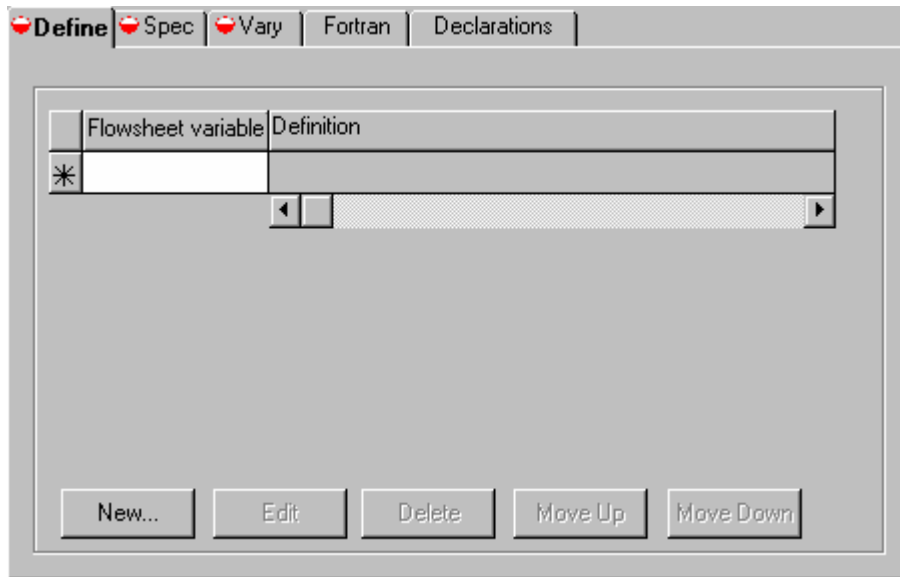
Defining the Design Specification

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 98.0%.

To Enter Design Specifications

- 1 Select **Data | Flowsheeting Options | Design Spec.**
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 **Flowsheeting Options | Design Spec | 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 DS-1, you will copy it from the Sensitivity.

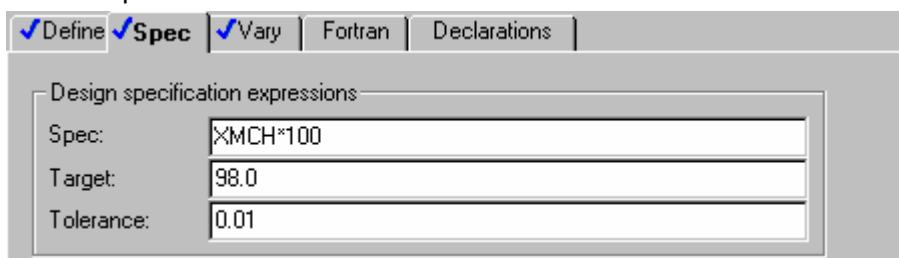
- 1 In the Explorer pane of the Data Browser, expand **Model Analysis Tools, Sensitivity, and S-1**.
- 2 Click the **Input** form under **S-1**. The **Define** sheet for Sensitivity S-1 appears.
- 3 Select **XMCH**, and click **Copy**.
- 4 Click **Input** under **Design Spec DS-1**. The **Define** sheet for Design-Spec DS-1 appears.
- 5 Click **Paste**. Variable XMCH has been copied to Design-Spec DS-1. The **Flowsheeting Options | Design Spec | DS-1 | Input | 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 the **Spec** tab. The **Flowsheeting Options Design Spec DS-1 Input 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 98.0.
- 4 In the **Tolerance** field, enter 0.01 to specify an acceptable deviation from the target percentage.


The completed sheet looks like this:



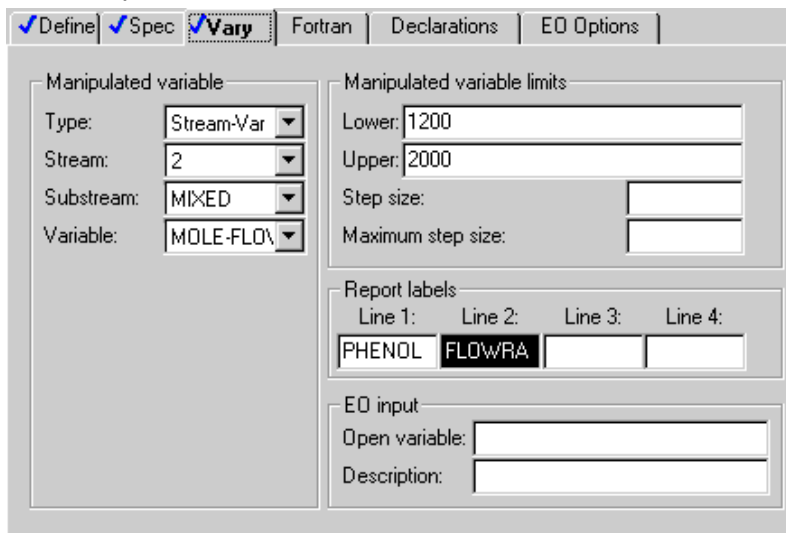
Design specification expressions	
Spec:	XMCH*100
Target:	98.0
Tolerance:	0.01

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 the **Vary** tab.
The **Flowsheeting Options | Design Spec | DS-1 | Input | Vary** sheet appears.
- 2 In the **Manipulated variable** area, click the **Type** field and select **Stream-Var**.
- 3 In the **Stream name** 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 screenshot shows the 'Vary' tab of the Aspen Plus Design Spec DS-1 form. The 'Manipulated variable' section has the following settings: Type: Stream-Var, Stream: 2, Substream: MIXED, and Variable: MOLE-FLOW. The 'Manipulated variable limits' section has Lower: 1200 and Upper: 2000. The 'Report labels' section has Line 1: PHENOL and Line 2: FLOWRA. The 'EO input' section has empty fields for Open variable and Description.

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

Select **Data | Model Analysis Tools | Sensitivity**. The **Sensitivity** Object Manager Appears.




Select row **S-1**, and click **Hide**. 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, the Reveal button will be active. Click the Reveal button 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 Aspen Plus menu bar, select **Run | Run**.
- From the Aspen Plus toolbar, click .
- Click  to open the Control Panel and then click  from the Control Panel.
- Press **F5**.

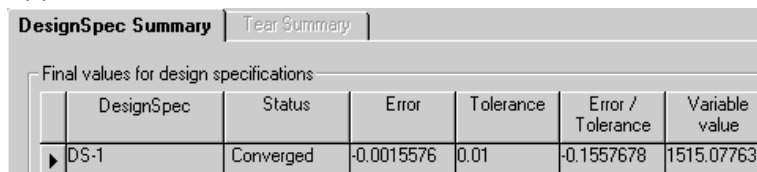
Then examine the results.

Examining Design Specification Results

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

- 1 From the Data Browser menu tree, click **Results Summary | Convergence**.

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



DesignSpec	Status	Error	Tolerance	Error / Tolerance	Variable value
DS-1	Converged	-0.0015576	0.01	-0.1557678	1515.07763

The results show that the calculation converged successfully and that the necessary value of the phenol flow rate is approximately 1517.1. 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 **Aspen Plus** menu bar, click **File | Exit**.
The **Aspen Plus** dialog box appears.
- 2 Click **Yes** to save the simulation.

5 Creating a Process Flow Diagram

Aspen Plus has two modes for displaying graphics:

- Simulation mode
- PFD (Process Flow Diagram) mode

In both modes, you can modify your process flowsheet to prepare customized drawings for reports by:

- Adding text and graphics
- Displaying global data for streams and blocks
- Displaying stream results tables
- Adding OLE objects

In PFD mode, you can modify the flowsheet to match your plant. For example, a single piece of equipment in the plant that is modeled by two unit operation blocks can be replaced by a single block in PFD mode. These changes are for display purposes and do not affect the flowsheet you developed to model your process.

In this chapter, you will use PFD mode to generate a plant diagram from 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 | Aspen Engineering Suite | Aspen Plus <version> | Aspen Plus User Interface**.

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

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 In the **Aspen Plus Startup** dialog box, make sure **Open an Existing Simulation** is selected.
 - 2 In the list, select **MCH.apw** and click **OK**.
- or-

If Your Saved File MCH.apw is not Displayed

- 1 In the **Aspen Plus Startup** dialog box, make sure **Open an Existing Simulation** is selected.
- 2 In the list box, double-click **More Files**, or click **OK** without selecting anything in the list box.
The **Open** dialog box appears.
- 3 Navigate to the directory containing your saved **MCH.apw** or navigate to the **Examples** 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.

- 4 Select either **MCH.apw** or **MCH.bkp** and click **Open**.

Note: If the **Connect to Engine** dialog box appears, see "[Connecting to the Aspen Plus Simulation Engine](#)" on page 93.

The **Process Flowsheet** window for the MCH simulation appears.

Switching to PFD Mode

Simulation mode is the Aspen Plus default mode that you use to model a process or perform calculations. PFD mode is used to create a graphical representation of your process for a report or for display purposes. Use PFD mode to do the following:

- Add equipment icons and streams that were not explicitly included in the simulation.
- Display stream data.
- Display a results table.
- Add a title.

To toggle between Simulation Mode and PFD Mode, use either of the following methods:

- Select **View | PFD Mode**.
- Press **F12**.

The check mark next to **PFD Mode** in the **View** menu and the status bar at the bottom of the main window indicate that PFD mode is on. Also, the process flowsheet workspace has a thick colored border when you are using PFD mode.

When you select PFD mode, Aspen Plus creates a new graphic identical to the original flowsheet. This new graphic is independent of the original. Making changes to streams and blocks in either one and toggling modes will show that these changes do not cross over.



Note: If you change the original process flowsheet model and you wish to start over again with a new PFD style drawing that contains these changes, select **View | Reset PFD** while in PFD mode. Your old PFD will be deleted and it will be replaced by a new drawing identical to the process flowsheet from your revised simulation model.

Adding a Pump to the Diagram

In the MCH simulation, you did not model the feed pump to the column; instead, you simply specified the pressure in the feed stream. However, you may wish to include a feed pump in a drawing used for a report or display.

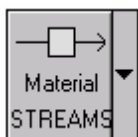
Place a pump in your diagram and split Stream 1 into two streams – one entering the pump and one leaving the pump and entering Block B1. Follow the directions below.

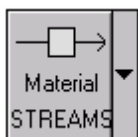
To Add the Feed Pump to the PFD Diagram

- 1 Enter PFD Mode by selecting **View | PFD Mode** if you have not already done so. Look for the colored border on the process flowsheet and the words *PFD Mode* in the bottom status bar to ensure you are in PFD Mode.
- 2 From the Model Library, click the **Pressure Changers** tab.
- 3 Click  next to the **Pump** unit operation model.
- 4 Hover over the icons to see their labels and select **ICON1**.
- 5 Drag (click and hold) the selected icon to the **Process Flowsheet** window to create Pump block B2.
- 6 Place the pump icon in the middle of Stream 1.
- 7 Click  to stop adding the unit operation model.

To Insert the Pump Into the Feed Stream

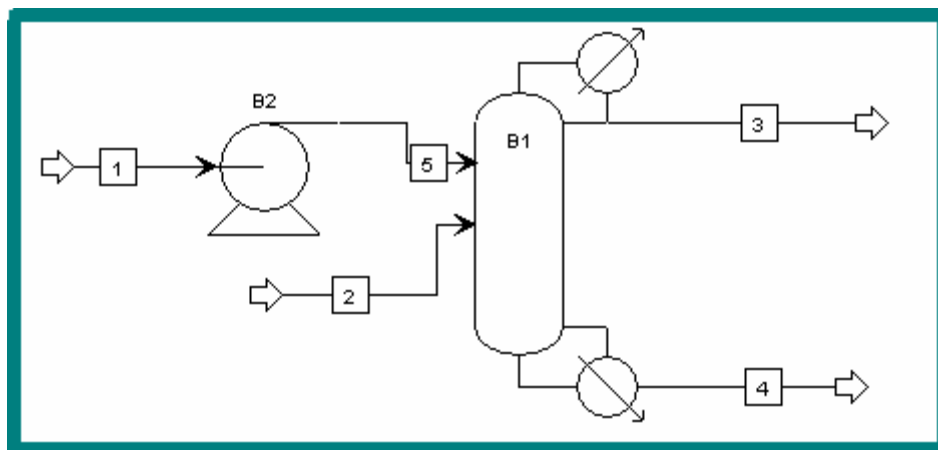
- 8 Select Stream 1 and right-click.
- 9 From the shortcut menu, select **Reconnect Destination**.
Stream 1 is now disconnected from Block B1 and you are ready to reconnect it to the pump.
- 10 Move the cursor arrowhead \blacktriangleright to an inlet port on the pump and left-click.
Stream 1 now enters the pump and you are ready to create a new stream from the pump to Block B1.



- 11 Click once on  on the left side of the Model Library.
- 12 Move the cursor (now a crosshair \oplus) to an outlet port on the pump and click once.
- 13 Move the cursor (now an arrowhead \blacktriangleright) to a feed port on Block B1 and click once to create a fifth stream.

Note: To cancel connecting the stream at any time, press **ESC**.

Your diagram should look something like this:



The Block names B1 and B2 have been moved for clarity. If you wish, you may also rename Stream 5 to Stream 1 or Stream 1A since the pump doesn't change the components of the stream.

Once you are satisfied with the layout, you can lock the existing layout to prevent accidental movement of blocks or streams.

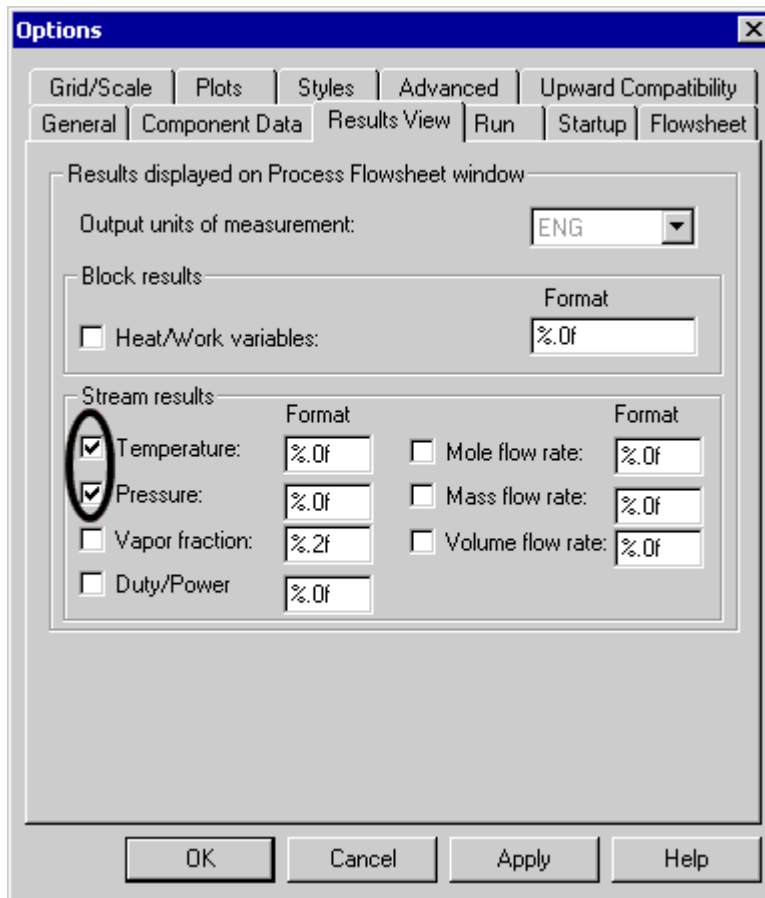
From the Flowsheet pulldown menu, select Lock. Locking the flowsheet applies to both PFD mode and normal mode.

Note: If you make a mistake while working with the graphics, it is easy to Undo the mistake. From the **Edit** menu, select **Undo**. The Undo only applies to the graphical flowsheet (placing a block, moving a stream, etc.). Due to limitations in the GUI architecture, the Undo button cannot be used to Undo changes to the forms.

Displaying Stream Data

To Display Temperature and Pressure

- 1 From the **View** menu, ensure that **Global Data** has a checkmark next to it.
- 2 Select **Tools | Options | Results View**.
- 3 Select the **Temperature** and **Pressure** checkboxes.

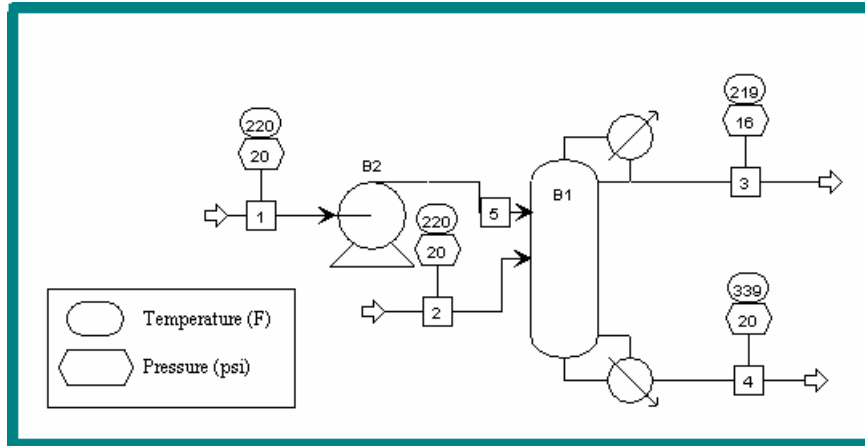


- 4 Click **OK**.

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 Full** or press **Ctrl-End** to see the whole drawing.

Your diagram should look approximately like this:



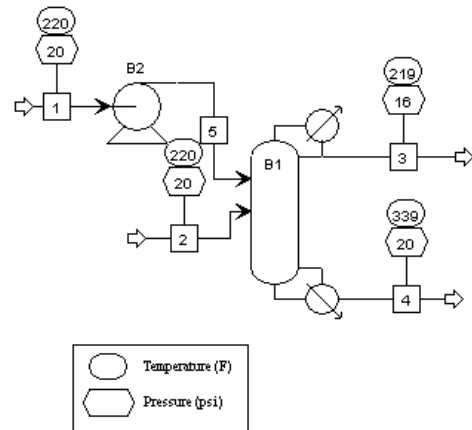
Adding a Stream Table

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

- 1 From the **View** menu, ensure **Annotation** is selected.
- 2 Select **Data | Results Summary | Streams**.
The **Results Summary | Streams | Material** sheet appears with data from all streams displayed.
- 3 Click **Stream Table** to place the table on your diagram.
- 4 Click the **Process Flowsheet** tab to return to your diagram.

A birdcage-style stream table appears in the **Process Flowsheet** window 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 to display the shortcut menu.
- 4 From the shortcut menu, select **Zoom In**.

Adding Text


Add a title to the drawing using the **Draw** toolbar.

To Display the Draw Toolbar

- 1 Select **View | Toolbar**.
- 2 In the **Toolbars** dialog box, select the **Draw** checkbox.
- 3 Click **OK**.

The **Draw** toolbar appears.

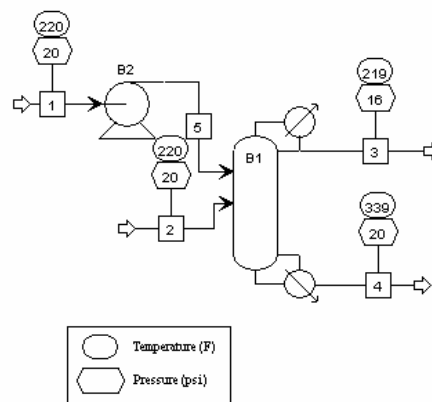
To Add Text

- 4 From the **Draw** toolbar, click .
- 5 Move the cursor to an appropriate spot for the text and left-click.
A rectangular box with a blinking cursor appears.
- 6 Type **Methylcyclohexane Recovery Column**, then click outside the rectangular box.
- 7 Select the title and change the font size to 28 using the **Draw** toolbar.
- 8 Click the title and hold the mouse button down until the cursor changes shape, then drag the title anywhere you like.
- 9 Select **View | Zoom Full**.

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	23.380



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 | Annotating Process Flowsheets**.

To Preview Your Drawing Before Printing

- 1 Select **File | Print Preview**.

The block and stream IDs and the global data in your drawing are now scaled approximately as they will appear in print.

- 2 Click **Zoom In** or **Zoom Out**.

To Print the PFD-Style Drawing

- 3 Click **Print**.

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

- 4 Select the appropriate printer and click **OK**.

Leaving PFD Mode

You have seen how straightforward it is to create a PFD-style drawing from a process flowsheet. Remember that the modifications you have made for the PFD-style drawing have no effect on the process flowsheet and will not be included in it.

To Return to Simulation Mode

- 1 Select **View | PFD Mode** or press **F12** to toggle PFD mode off and return to simulation mode.
The original process flowsheet is displayed without the pump, but with the stream pressure and temperature data, the results table, and the title that you added in PFD mode.
- 2 Select **View | Global Data** to toggle it off if you don't want to view the table and the pressure and temperature data in the original process flowsheet.
- 3 Select **View | Annotation** to toggle it off if you don't want to view the title in the original process flowsheet.

Note: Remember, the streams and blocks in the PFD drawing and the process flowsheet are independent of one another unless you select **View | Reset PFD** while in PFD mode.

Exiting Aspen Plus

- 1 Select **File | Exit**.
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.

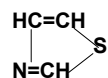
Allow about 30 minutes for this simulation.

Thiazole Physical Property Data

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

Thiazole (C₃H₃NS) 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 | Aspen Engineering Suite | Aspen Plus <version> | Aspen Plus User Interface**.
The **Aspen Plus Startup** dialog box appears.
- 3 From the **Aspen Plus Startup** dialog box, select **Template** and click **OK**.
The **New** dialog box appears.

Creating a Property Estimation Simulation

Use the **New** dialog box to specify the application type and the run type for the new simulation.

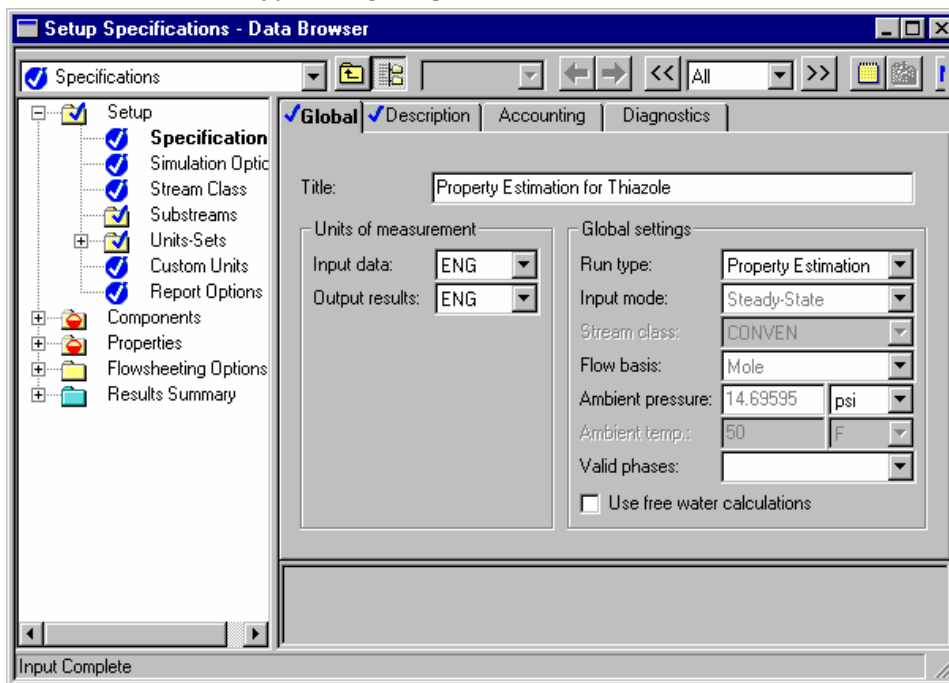
- 1 From the **New** dialog box, select the **General with English Units** application type.
- 2 In the **Run Type** field, click and select **Property Estimation**.
- 3 Click **OK**.

Note: If the **Connect to Engine** dialog box appears, see "[Connecting to the Aspen Plus Simulation Engine](#)" on page 93.

The Data Browser appears. There is no 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.

Entering a Title

- 1 Expand the **Setup** folder in the Data Browser menu tree and click **Specifications**.
The **Setup | Specifications | Global** sheet appears. The run type *Property Estimation* is already selected.
- 2 In the **Title** field, type **Property Estimation for Thiazole**.



Next, define a component called THIAZOLE.

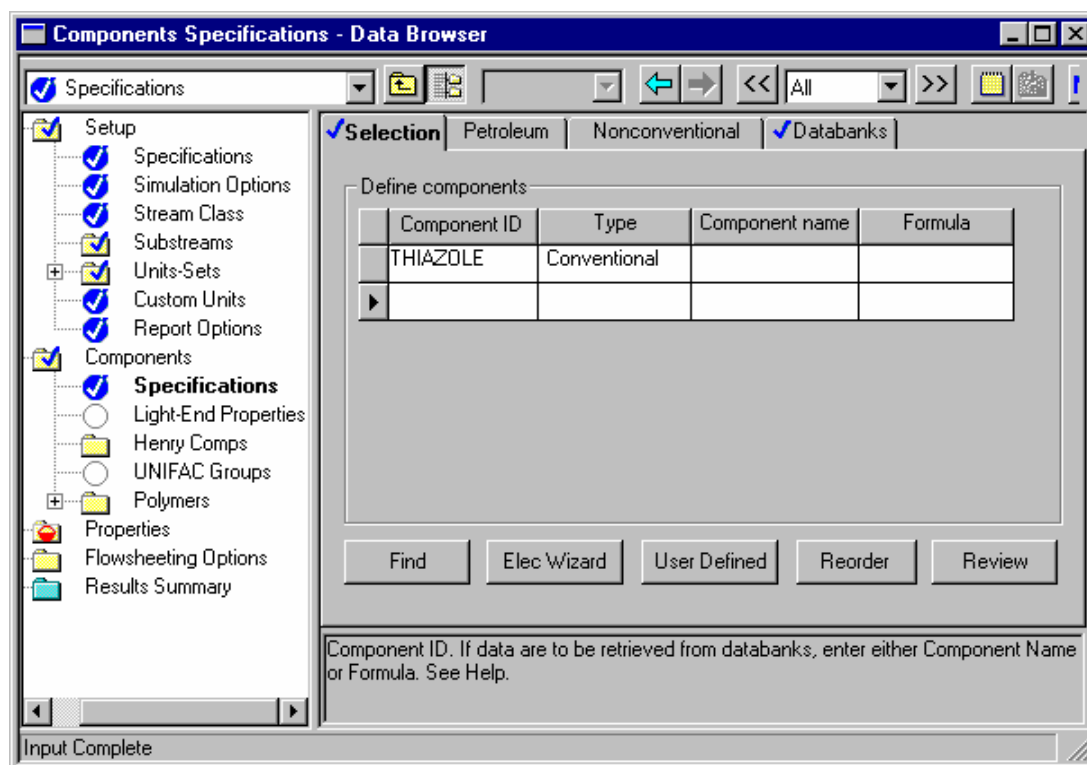
Entering Components Information

- 1 Expand the **Components** folder in the Data Browser menu tree and click **Specifications**.

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

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

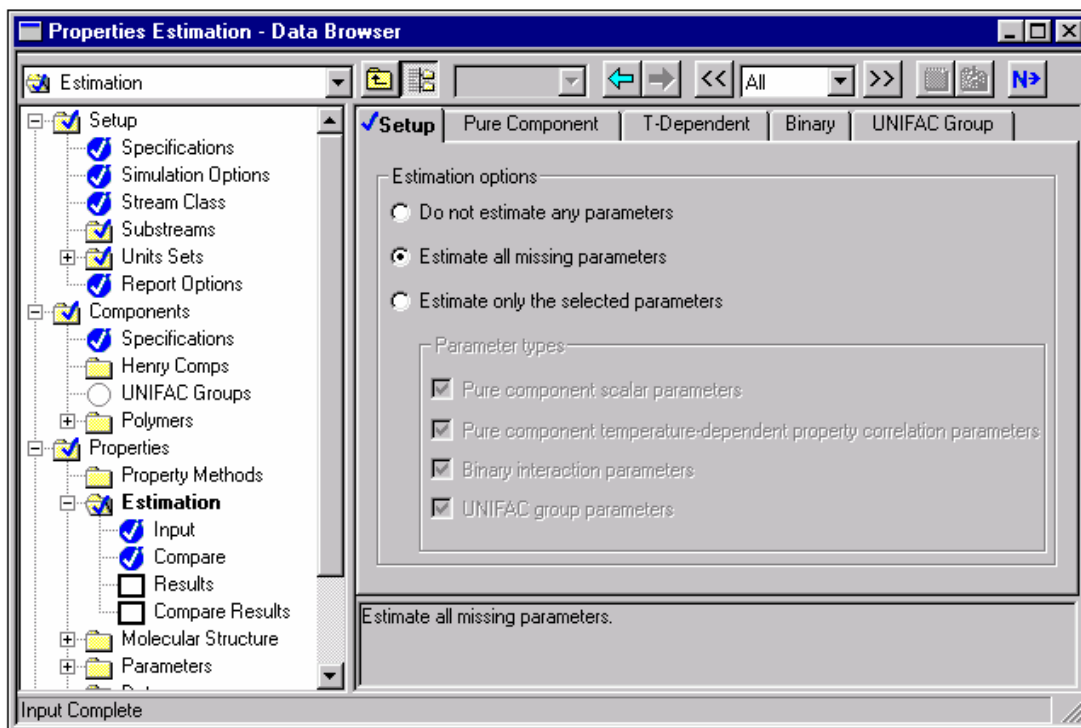
Because THIAZOLE is not in the Aspen Plus databank, do not fill in the **Component name** or **Formula** columns.



Next, tell Aspen Plus to estimate all missing properties.

Specifying Properties to Estimate

- 1 Expand the **Properties** folder and the **Estimation** folder and click **Input**. The **Properties Estimation Input Setup** sheet appears.
- 2 Accept the default Estimation option **Estimate all missing parameters**.



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. Click .

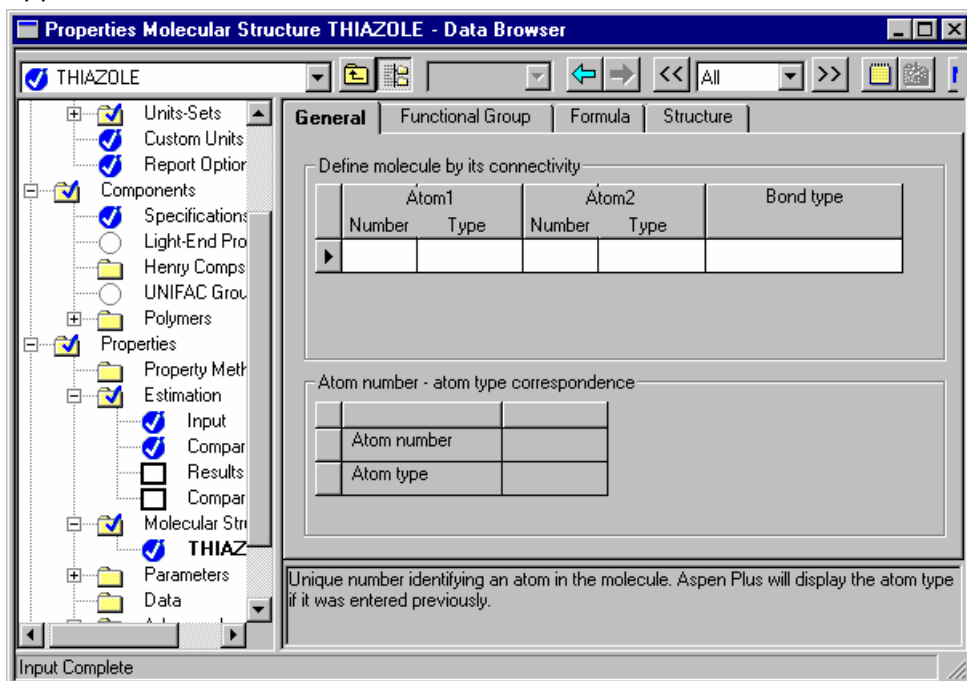
Entering Molecular Structure

The **Non-Databank Components** dialog box appears, indicating that your simulation has some non-databank components, for which you can enter additional information.

To Enter the Molecular Structure Information for Thiazole

- 1 Click **Cancel**.
- 2 Expand the **Properties | Molecular Structure** folder in the Data Browser menu tree and click **THIAZOLE**.

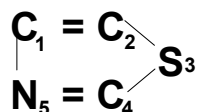
The **Properties | Molecular Structure | THIAZOLE | General** sheet appears:



Note: You can define the molecular structure either 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. This example explains how to use the General Method.

On the **General** sheet, specify the molecular structure of Thiazole by listing each non-hydrogen atom and each bond. Aspen Plus handles the hydrogen.

- 3 Sketch the structure of Thiazole and number all the non-hydrogen atoms:



Each atom will be listed twice, once as an atom that *connects* (Atom 1) and once as an atom that *is connected to* (Atom 2).

- 4 Enter the following information for **Atom 1**:

Number	Type
1	C
2	C
3	S
4	C
5	N

This table associates each number with type of atom.

- 5 Enter the following information for **Atom 2**:

Number	Type (generated automatically)
2	C
3	S
4	C
5	N
1	C

This table indicates which atom is connected to each of the atoms in the first table.

- 6** In the **Bond type** column, select *Double bond* between atoms 1 and 2 and between 4 and 5, and select *Single bond* for the other bonds.

The **Properties Molecular Structure THIAZOLE General** sheet is now complete:

Define molecule by its connectivity					
Atom1		Atom2		Bond type	
Number	Type	Number	Type		
1	C	2	C	Double bond	
2	C	3	S	Single bond	
3	S	4	C	Single bond	
4	C	5	N	Double bond	
5	N	1	C	Single bond	
*					

Atom number - atom type correspondence					
Atom number	1	2	3	4	5
Atom type	C	C	S	C	N

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 **Properties | Parameters** folder in the Data Browser menu tree and click **Pure Component**.

The **Properties | Parameters | Pure Component** object manager appears.

- 2 Click **New**.
- 3 In the **New Pure Component Parameters** dialog box, select **Scalar**.
- 4 Enter the new name TBMW (for boiling point and molecular weight) and click **OK**.
The **Properties | Parameters | Pure Component | 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.

Pure component scalar parameters					
	Parameters	Units	Data set	Component	Component
	TB	C	1	THIAZOLE	
▶	MW		1	85	
*					


Next specify the coefficients for the Antoine vapor pressure correlation.

To Enter Antoine Vapor Pressure Correlation Coefficients

- 1 Click **Properties | Parameters | Pure Component** in the Data Browser menu tree.
The object manager appears. You can see that you have filled your TBMW parameter 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.
- 4 Under **Liquid Vapor Pressure**, select **PLXANT-1** for the Antoine vapor pressure correlation.
- 5 Click **OK**.
The **Properties | Parameters | Pure Component | 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 $69\text{ °C} < T < 118\text{ °C}$.

You can get help on specifying the coefficients by clicking , then clicking PLXANT in the **Parameter** field near the top of this sheet. Follow the link to [Extended Antoine/Wagner](#).

- 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 Properties Parameters Pure Component PLXANT-1 Input sheet:

✓ Input


Parameter: Data set:


Temperature-dependent correlation parameters

Components	<input type="text" value="THIAZOLE"/>	<input type="text"/>
▶ Temperature units	C	
Property units	mmHg	
1	16.445	
2	-3281	
3	216.255	
4	0	
5	0	
6	0	
7	0	
8	69	
9	118	

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)

1 Select **View | Control Panel** or press **F7** or press the control panel button  on the Aspen Plus toolbar.

2 Select **Run | Run** or press **F5** or press the run button  to run the estimation.

As the run executes, status messages display in the **Control Panel**. 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 In the Data Browser menu tree, click **Results Summary | Run Status**.
A summary sheet appears indicating that the calculations were completed with warnings.
- 2 In the Data Browser menu tree click, **Properties | Estimation | Results**.
The **Pure Components** sheet appears, with the estimated pure component properties for Thiazole. The property name, abbreviation, estimated value, units, and method used for estimation are tabulated.

Pure Component					
T-Dependent		Binary	UNIFAC Group		
Component:	THIAZOLE	Formula:	C3H3NS		
Estimated pure component parameters					
PropertyName	Parameter	Estimated value	Units	Method	
CRITICAL TEMPERATURE	TC	632.471008	K	JOBACK	▲
CRITICAL PRESSURE	PC	6653023.53	N/SQM	JOBACK	■
CRITICAL VOLUME	VC	0.2125	CUM/KMOL	JOBACK	
CRITICAL COMPRES.FAC	ZC	0.26885004		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	169180000	J/KMOL	JOBACK	
STD.FREE ENERGY FORM	DGFORM	195470000	J/KMOL	JOBACK	
ACENTRIC FACTOR	OMEGA	0.23792659		DEFINITI	
HEAT OF VAP AT TB	DHVLB	36210627	J/KMOL	DEFINITI	
LIQUID MOL VOL AT TB	VB	0.07844136	CUM/KMOL	GUNN-YAM	
SOLUBILITY PARAMETER	DELTA	23340.0458	(J/CUM)**.5	DEFINITI	
UNIQUAC R PARAMETER	GMUQR	2.72972973		BONDI	
UNIQUAC Q PARAMETER	GMUQQ	1.816		BONDI	▼

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:

Pure Component | **T-Dependent** | Binary | UNIFAC Group

Component: THIAZOLE Formula: C3H3NS

Estimated T-dependent parameters

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		
		0.14817965		
		2.16490922		
HEAT OF VAPORIZATION	DHVLWT	38893138.7	K,J/KMOL	DEFINITI
		342.15		
		0.32051562		
		0.20012116		

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**
- 2 In the **Save As** dialog box, select *Aspen Plus Backup Files* in the **Save as type** field.
- 3 In the **File Name** field, enter **thiazole**.
- 4 Click **Save**.

An **Aspen Plus** dialog box appears warning you that you will not be able to start new calculations from previous results and suggests saving the file as an Aspen Plus document file (.apw).

- 5 Click **No** since you only need the backup file.

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.
- 2 Click **File | Import** and select **thiazole.bkp** and click **Open**.

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

- 3 An **Information** dialog box appears. Click **OK**.
The flowsheet disappears since the thiazole backup file is a properties estimation. However, the flowsheet data from **Flash.apw** is still available.
- 4 Press **F8** to open the Data Browser.
- 5 In the Data Browser menu tree expand the **Setup** folder and click **Specifications**.
The **Setup | Specifications | Global** sheet appears.
- 6 In the Global Settings area, change the run type to **Flowsheet**.
The flowsheet and stream and block input data from **Flash.apw** are now accessible.
- 7 In the Data Browser menu tree, click **Properties | Estimation | Input** and then select **Do not estimate any parameters** since the thiazole parameters have already been estimated.
- 8 In the Data Browser menu tree, 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.
- 9 Press **F5** to run the simulation with thiazole in Stream 1.

Exiting Aspen Plus

- 1 Select **File | Exit**.
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 | Aspen Engineering Suite | Aspen Plus <version> | Aspen Plus User Interface**.
The **Aspen Plus Startup** dialog box appears.
- 3 Select **Template** and click **OK**.
The **New** dialog box appears.
- 4 Select **General with English Units** for the application type.
- 5 In the **Run Type** field, click  and select **Property Analysis**.
- 6 Click **OK**.

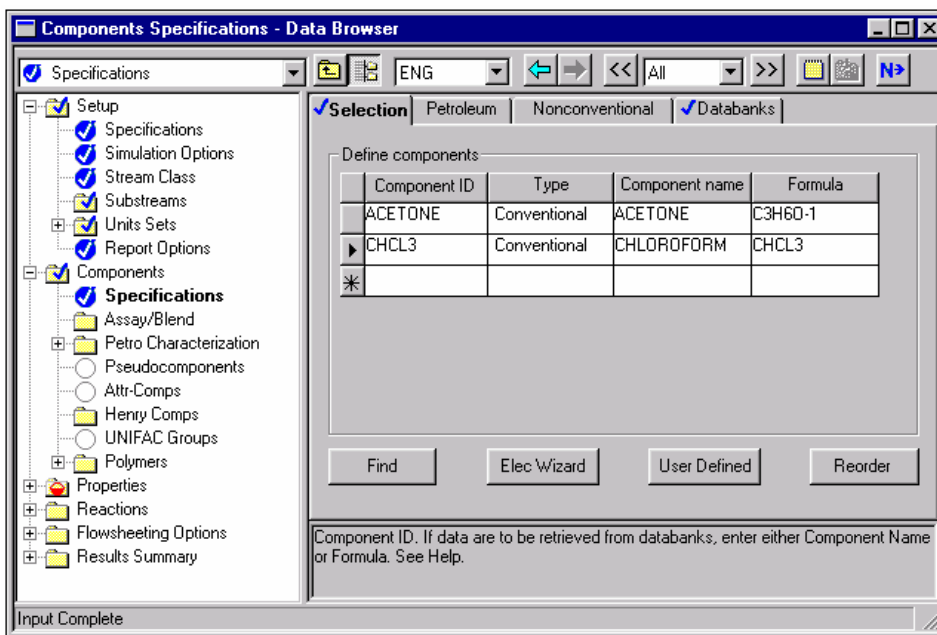
Note: If the **Connect to Engine** dialog box appears, see "[Connecting to the Aspen Plus Simulation Engine](#)" on page 93.

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


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 Click .
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 In the **Input data** field, click  and select **METCBAR** for METric units with Celsius for temperature and BAR for pressure.
- 4 Click  to continue.
The **Components | Specifications | Selection** sheet appears.
- 5 In the first line under the **Component ID** field, type ACETONE and press **Enter** on the keyboard.
- 6 In the second line under the **Component ID** field, type CHCL3 for chloroform and press **Enter** on the keyboard:



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

- 7 Click  to continue.

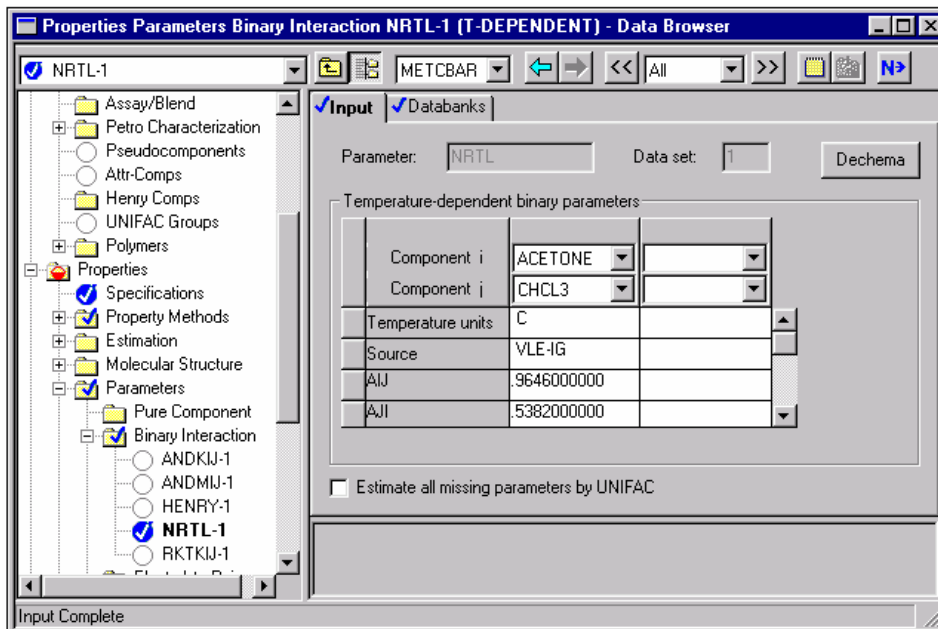
The **Properties | Specifications | Global** sheet appears.

For this simulation, use the NRTL physical property model to generate the vapor-liquid equilibrium properties.

- 8 In the **Base method** field, click  and select **NRTL**.

- 9 Click  to continue.

The **Properties | Parameters | Binary Interaction | NRTL-1 | 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 15° C and 64.47° C.

Examine additional information on the range of data used and the quality of the fit by using the online help.

- 10 Place the cursor in one of the fields containing a numerical value.
11 Press **F1**.

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

Databank: VLE-IG		Parameter: NRTL		
Components: C3H6O-1, CHCL3				
Range of data used in Data Regression:				
State variable	Range			
Temperature, C	15.0000 - 64.4700			
Pressure, mmHg	101.0000 - 760.0000			
Liquid mole fraction (C3H6O-1)	0.00810 - 0.99810			
Residual root mean squares error: 20.6330				
Average deviations:				
State variable	No. points	Relative %	Absolute	Maximum
Temperature, C	127	0.310000	0.200000	-0.380000
Pressure, mmHg	311	0.480000	1.740000	7.370000
Vapor mole fraction	316	2.946813	0.006392	0.046701

- 13 Press **Enter** on the keyboard.

- 14 Click  to continue.

An **Information** dialog box appears telling you that you have to specify the property analysis to be generated. Because you will perform an ad-hoc property analysis in this simulation, you need not continue with the next simulation input.

- 15 Click **Cancel** to close the dialog box.

Generating a Txy Diagram

You can use the Aspen Plus analysis capability before input specifications are complete. Note the *Required Input Incomplete* 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 Aspen Plus menu bar, select **Tools | Analysis | Property | Binary**.

The **Binary Analysis** dialog box appears.

- 2 In the **Analysis type** field, click to view the types of analysis available.

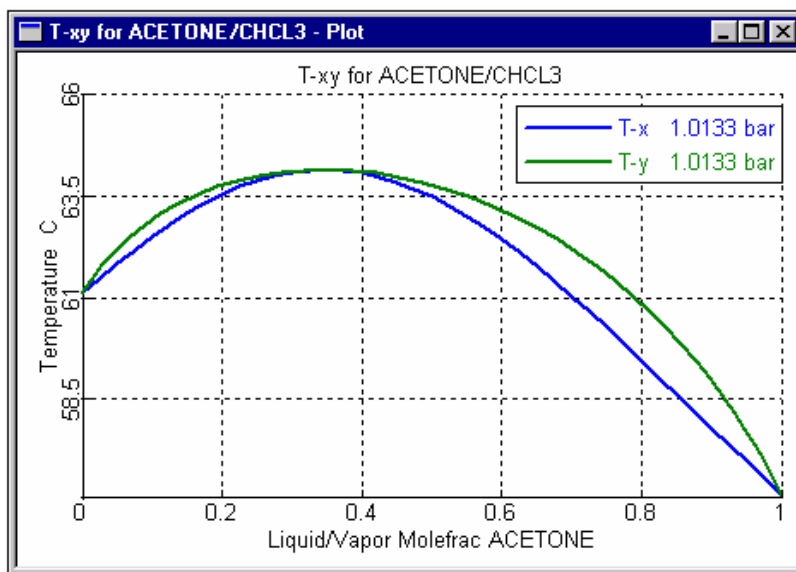
As the prompts indicate, Txy and Pxy analysis are used to study nonideality of vapor-liquid systems to check for azeotrope formation. Gibbs energy of mixing analysis is used to see if the system will form two liquid phases.

- 3 Select **Txy**.

The fields in this dialog box are filled with default options all of which are correct for this example.

- 4 Click **Go** to apply the defaults and start the analysis.

Calculations begin for the T-xy diagram. When the calculations are finished, the results appear in tabular form. In addition, a T-xy plot is automatically displayed, as shown in the following figure:



- 5 Click to obtain a maximized plot screen.

Clicking inside the plot will reveal the coordinates of the cursor. 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.

- 6 Select the **Binary Analysis Results** window which is behind the **Plot** window.

The table shows that Aspen Plus has calculated activity coefficients 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 using the Plot Wizard.

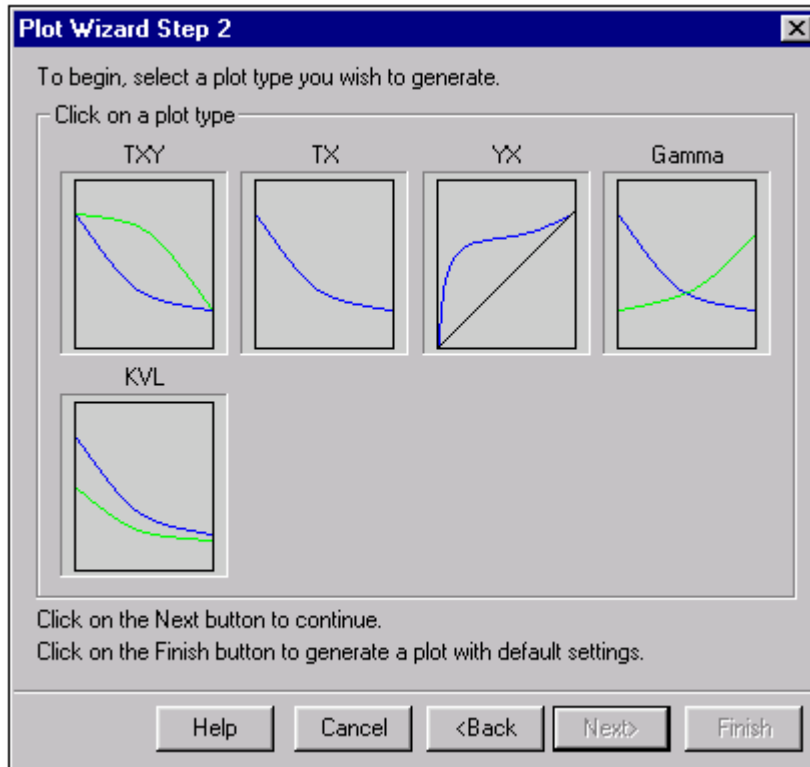
To Generate an Activity Coefficient Plot

7 In the **Binary Analysis Results** window, click **Plot Wizard**.

The **Plot Wizard Step 1** window appears.

8 Read the description on the page and click to continue.

The **Plot Wizard Step 2** window appears with the available plots.



9 Select **Gamma** to plot activity coefficients versus mole fraction of acetone.

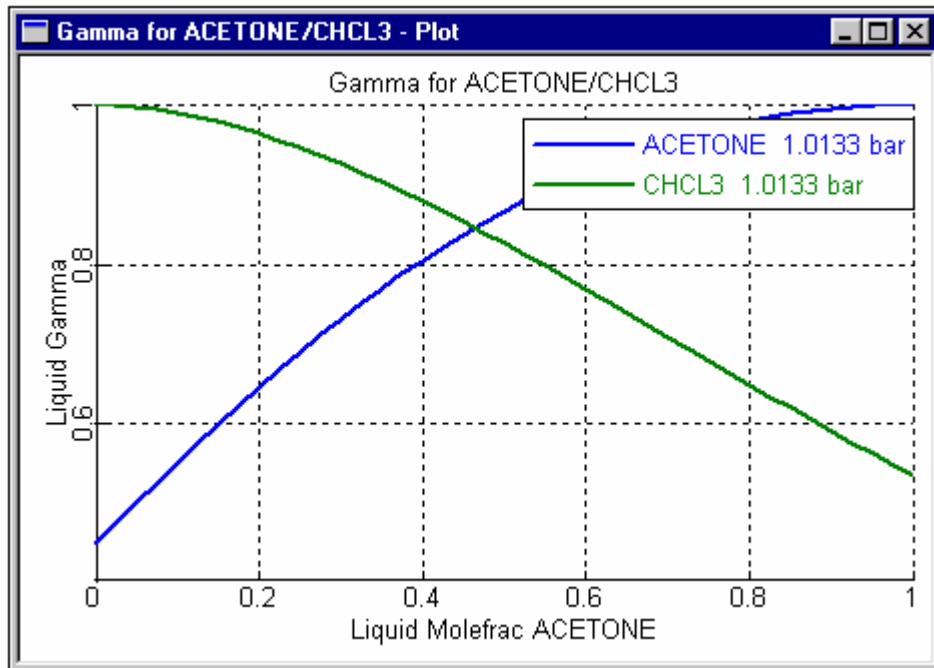
10 Click to continue.

The **Plot Wizard Step 3** window appears.

11 In the **Component to plot** field, click and select **ACETONE**.

12 Click **Finish** to accept defaults for the remaining plot settings and generate the plot.

The activity coefficient plot appears:



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

13 Close the **Plot** and **Binary Analysis Results** windows.

Note: In the **Binary Analysis** dialog box, you can click **Save as Form** to save your interactive property analysis to forms within the Data Browser. Saving an interactive property analysis as forms enables you to preserve the input and results of this property analysis to view or modify at a later time.

14 Close the **Binary Analysis** dialog box.

At this point you could change the run type in the **Setup Specifications Global** sheet to Flowsheet, define a flowsheet, and proceed with a simulation. However, for this simulation, stop here.

15 From the **File** menu, select **Exit**.

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

8 Connecting to the Aspen Plus Simulation Engine

If either of the following conditions exist, you will be prompted to specify the host computer for the Aspen Plus simulation engine after you start the Aspen Plus User Interface:

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

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

- 1** In the Server type field, click and select the type of host computer for the simulation engine.
- 2** If you choose *Local PC* as the server for the simulation engine, you do not need to enter any more information into the dialog box. Click **OK** to continue.

If you choose *Windows 2000 or XP server* as the server for the simulation engine, continue with the following steps.

- 3** In the **Node name** field, enter the node name of the computer on which the Aspen Plus simulation engine will execute.
- 4** In the other fields, enter the following information:

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

- 5** Click **OK**.

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

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