Aspen Plus®

STEADY STATE SIMULATION

Version 10

User Guide

AspenTech®

VOLUME 1

Use of Aspen Plus and This Manual

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Contents

About This Manual

The *Aspen Plus User Guide* consists of three volumes that provide step-by-step instructions for using Aspen Plus® to build and use a process simulation model.

Volume 1 describes the Aspen Plus user interface and explains how to perform the basic tasks for creating and running simulations. Topics include:

- Creating a simulation model
- Defining the flowsheet
- Entering the required information, such as components, streams and physical property data
- Running the simulation
- Examining results

Volume 2 contains procedures for using additional Aspen Plus capabilities:

- Convergence
- Sensitivity
- Design specifications
- Optimization
- Property analysis
- Data regression

Volume 3 contains information about:

- Pressure relief calculations
- Stream libraries
- Working with other Windows™ programs
- The Aspen Plus ActiveX® automation interface

For More Information

Online Help Aspen Plus has a complete system of online help and context-sensitive prompts. The help system contains both context-sensitive help and reference information. For more information about using Aspen Plus help, see the *Aspen Plus User Guide*, Chapter 3.

Aspen Plus Getting Started Building and Running a Process Model This tutorial includes several hands-on sessions to familiarize you with Aspen Plus. The guide takes you step-by-step to learn the full power and scope of Aspen Plus.

Aspen Plus Getting Started Modeling Processes with Electrolytes This tutorial includes several hands-on sessions to familiarize you with simulating electrolyte systems with Aspen Plus.

Aspen Plus Getting Started Modeling Petroleum Processes This tutorial includes several hands-on sessions to familiarize you with simulating petroleum processes with Aspen Plus.

Aspen Plus Getting Started Customizing Unit Operation Models This tutorial includes several hands-on sessions to familiarize you with the customization of unit operation models with Aspen Plus.

Aspen Plus User Guide The three-volume *Aspen Plus User Guide* provides step-by-step procedures for developing and using an Aspen Plus process simulation model. The guide is task-oriented to help you accomplish the engineering work you need to do, using the powerful capabilities of Aspen Plus.

Aspen Plus reference manual series Aspen Plus reference manuals provide detailed technical reference information. These manuals include background information about the unit operation models and the physical properties methods and models available in Aspen Plus, tables of Aspen Plus databank parameters, group contribution method functional groups, and a wide range of other reference information. The set comprises:

- *Unit Operation Models*
- *Physical Property Methods and Models*
- *Physical Property Data*
- *User Models*
- *System Management*
- *System Administration*
- *Summary File Toolkit*

Aspen Plus application examples A suite of sample online Aspen Plus simulations illustrating specific processes is delivered with Aspen Plus.

Aspen Plus Installation Guides These guides provide instructions on platform and network installation of Aspen Plus. The set comprises:

- *Aspen Plus Installation Guide* for Windows
- *Aspen Plus Installation Guide* for OpenVMS
- *Aspen Plus Installation Guide* for UNIX

The Aspen Plus manuals are delivered in Adobe portable document format (PDF) on the Aspen Plus Documentation CD.

Technical Support

World Wide Web For additional information about AspenTech products and services, check the AspenTech World Wide Web home page on the Internet at:

http://www.aspentech.com/

Technical resources To obtain in-depth technical support information on the Internet, visit the Technical Support homepage. Register at:

http://www.aspentech.com/ts/

Approximately three days after registering, you will receive a confirmation e-mail and you will then be able to access this information.

The most current Hotline contact information is listed. Other information includes:

- Frequently asked questions
- Product training courses
- Technical tips

AspenTech Hotline If you need help from an AspenTech Customer Support engineer, contact our Hotline for any of the following locations:

If you are located in:	Phone Number	Fax Number	E-Mail Address
North America & the Caribbean	+1-617/949-1021 +1-888/996-7001 (toll free)	+1-617/949-1724	support@aspentech.com
South America			
(Argentina office)	+54-11/4393-5308	+54-11/4394-8621	tecnoba@aspentech.com
(Brazil office)	+55-11/5506-0756	+55-11/5506-0567	tecnosp@aspentech.com
Europe, Gulf Region, & Africa			atesupport@aspentech.com
(Brussels office)	+32-2/724-0100	+32-2/705-4034	
(UK office)	+44-1223/312220	+44-1223/366980	
Japan	+81-3/3262-1743	+81-3/3262-1744	atjsupport@aspentech.com
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1 The User Interface

This chapter provides basic information on the Aspen Plus user interface. For information on how to use Aspen Plus to create a simulation model, see Chapter 2. If you are new to Aspen Plus, do the exercises in *Aspen Plus Getting Started Building and Running a Process Model* before using this manual.

This chapter explains the following topics:

- Starting Aspen Plus
- Aspen Plus windows
- Displaying, browsing, and completing forms
- Using Next—the Expert Guidance System

For more information on getting help on buttons, menus and other screen items, see Chapter 3.

Starting Aspen Plus

To start Aspen Plus:

1. Click Start, and then point to Programs
2. Point to AspenTech, point to Aspen Plus and then click Aspen Plus User Interface.
3. In the startup dialog box, choose whether you want to create a new simulation using a blank simulation or a Template, or open an existing simulation.

   If you choose to create a new run from a Template, you will be prompted to specify the Template and Run Type for the new run . See Chapter 2 for more information on creating a new run.

   Perform the remaining steps only if you are opening an existing run.
4. To open an existing simulation, either select the filename from the list in the startup dialog box, or select More Files, and click OK.

   If you select a file from the startup dialog box, the Aspen Plus main window appears with the chosen file displayed. If you choose More Files, the Open dialog box appears.

   Perform the remaining steps only if you chose More Files.
5. In the Open dialog box, in the Files of Type box, select the file format in which the run was saved. For example, Aspen Plus Document format (.apw) or Backup file format (.bkp). See Chapter 16 for more information on file formats and saving runs.
6. Use the Look In list box to locate the directory where the file is stored, then click the file you want to open, and click Open.

   If the Connect to Engine dialog box appears, see Connecting to the Aspen Plus Host Computer on page 1-3.

Tip To open an existing file quickly, just double-click the file from Windows Explorer.

Connecting to the Aspen Plus Host Computer

Use this section if:

- The Aspen Plus simulation engine is not installed on your PC
- The Aspen Plus simulation engine is installed on your PC and you are using the network license manager.

Skip this section if you are using the Activator security device on your PC.

These instructions assume that you are connected to the computer where the Aspen Plus simulation engine will run. See your Aspen Plus system administrator for information specific to your installation.

1. Start Aspen Plus and select a previous run, template, or blank simulation.

   The Connect to Engine dialog box appears.

2. Specify where the Aspen Plus engine will run:

Server Type	If the Aspen Plus engine runs on
Local PC	Your PC, using the network license manager
Unix host	A Unix server
OpenVMS host	An OpenVMS server
Windows NT server	A Windows NT server (Intel or AXP)

3. If you specified Unix host, OpenVMS host, or Windows NT server, enter the following information in the dialog box:

Enter this information	In this box
The type of Aspen Plus engine you want to connect to	Server Type
Node name of the computer the Aspen Plus simulation will run on	Node Name
Your logon name on the host computer	User Name
Password for your account on the host computer	Password
Working directory on the host computer for Aspen Plus runs	Working Directory

4. When the network connection is established, a message box appears saying Connection Established.

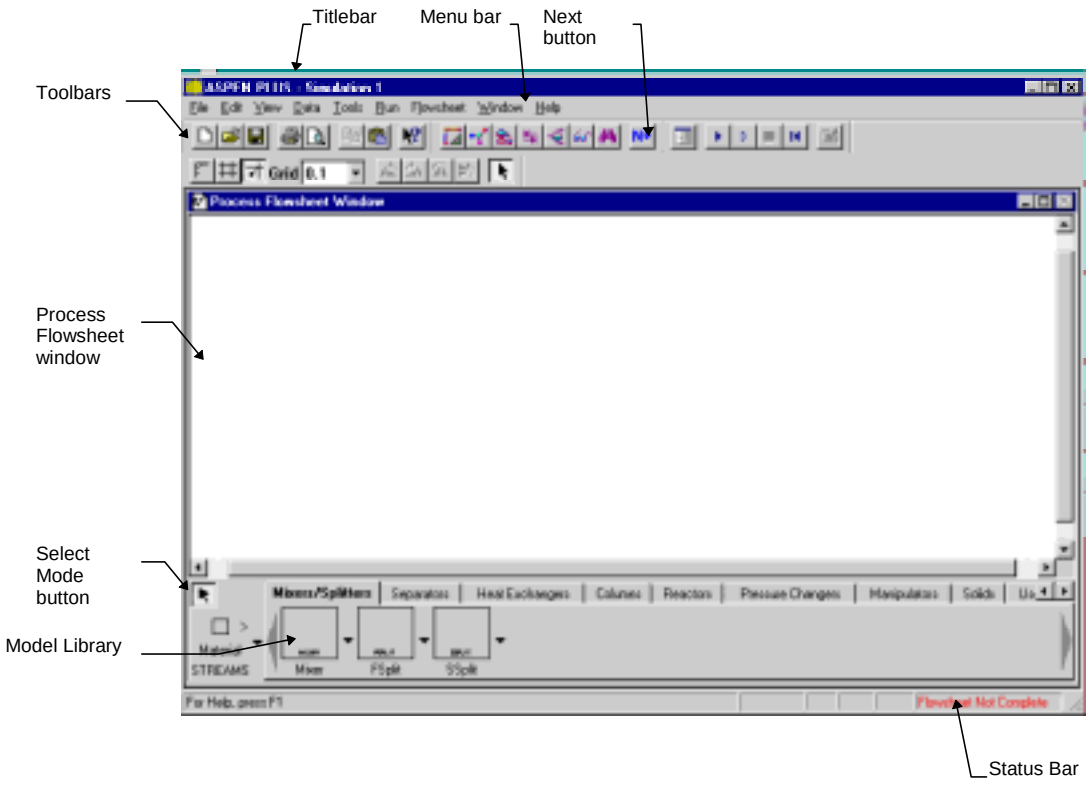
If the Connection Established box does not appear, see the Aspen Plus system administrator at your site for more information on network protocols and Aspen Plus host computers.

Tip It is possible to change the Connection by selecting Connect to Engine from the Run menu.

Tip You can specify additional host settings in the Settings dialog box. To do this, from the Run menu, click Settings.

The Aspen Plus Main Window

When you start Aspen Plus, the main window appears:



Use the workspace to create and display simulation flowsheets and PFD-style drawings. You can open other windows, such as Plot windows or Data Browser windows, from the Aspen Plus main window.

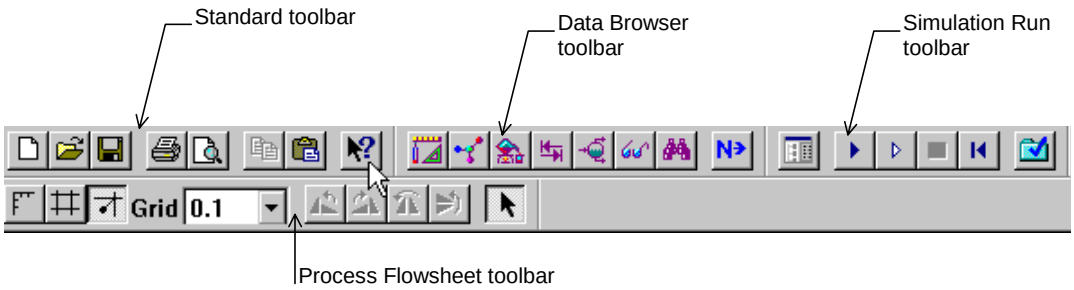
Tip You can display a window by selecting it from the Window menu. You can arrange the windows by selecting Tile or Cascade from the Window menu.

The parts of the Aspen Plus main window are:

Window Part	Description
Titlebar	Horizontal bar at top of window that displays the Run ID. Simulation 1 is the default ID until you give the run a name.
Menubar	Horizontal bar below the titlebar. Gives the names of the available menus.
Toolbar	Horizontal bar below the menubar. Contains buttons that when clicked, perform commands.
Next Button	Invokes the Aspen Plus expert system. Guides you through the steps required to complete your simulation.
Status Area	Displays status information about the current run.
Select Mode button	Turns off Insert mode for inserting objects, and returns you to Select mode.
Process Flowsheet Window	Window where you construct the flowsheet
Model Library	Area at the bottom of the main window. Lists available unit operation models.

Use the buttons on the toolbars to perform actions quickly and easily.

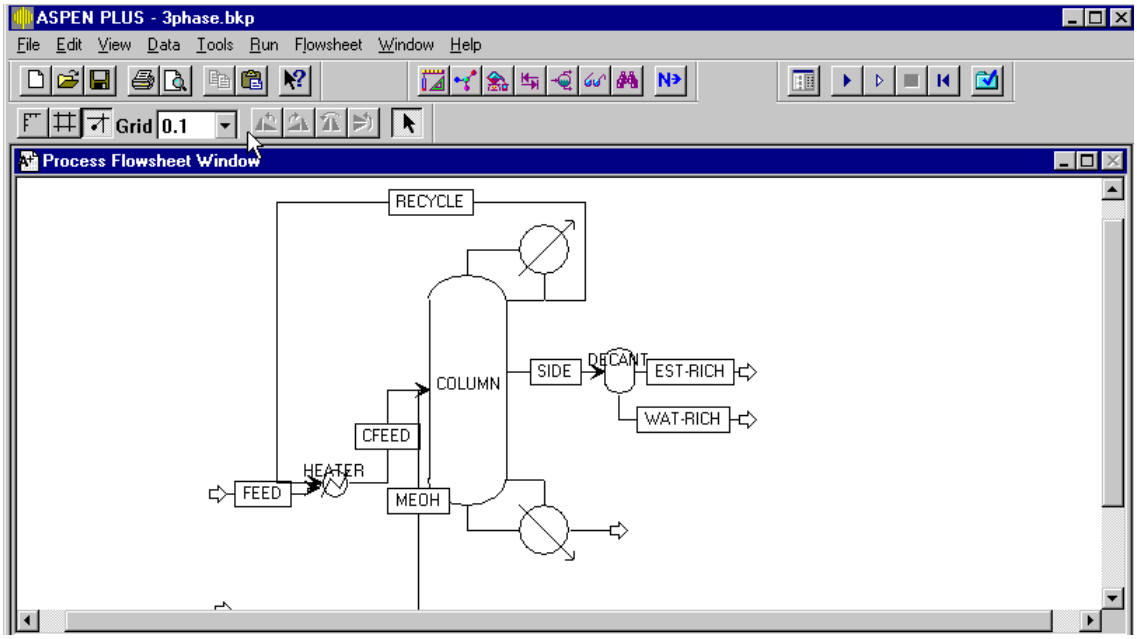
The default toolbars are shown here:



For information on viewing different toolbars, see chapter 16.

The Process Flowsheet Window

The Process Flowsheet window is where you create and display simulation flowsheets and PFD-style drawings.

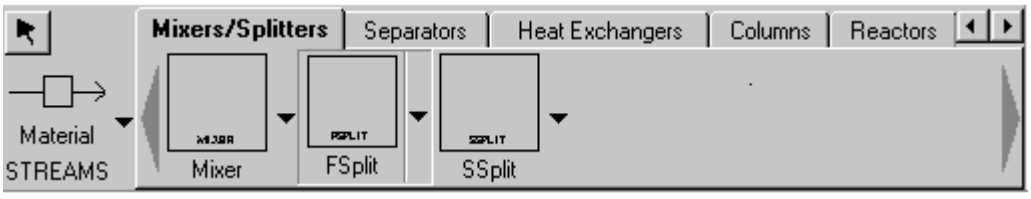


You can display the process flowsheet window in three different ways:

To display the Process Flowsheet window as	From the Window menu, click
A normal window	Normal
A window always in the background	Flowsheet as Wallpaper
A sheet of a workbook	Workbook mode

The Model Library

Use the Model Library to select unit operation models and icons that you want placed on the flowsheet. The Model Library appears at the bottom of the Aspen Plus main window.



To select a unit operation model:

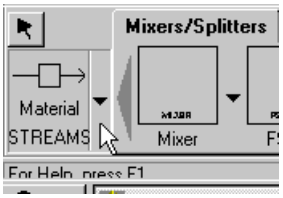
1. Click the tab that corresponds to the type of model you want to place in the flowsheet.
2. Click the unit operation model on the sheet.
3. To select a different icon for a model, click the down arrow next to the model icon to see alternate icons. The icon you select will appear for that model in the Model Library.
4. When you have selected a model, click the flowsheet where you want to place the model.

   When you place blocks this way, you are in Insert mode. Each time you click in the Process Flowsheet window, you place a block of the model type that you specified. To exit Insert mode and return to Select mode, click the Mode Select Button on the upper left of the Model Library.

Tip You can also place blocks in your flowsheet by dragging and dropping from the Model Library to the Process Flowsheet window.

To select the stream type:

1. Click the down arrow next to the stream type displayed in the Model Library.



2. Select the stream type you want to place in the flowsheet.
3. Once a stream type is selected, simply click the ports on the flowsheet where you want to connect the stream.

When placing blocks and streams, the mouse pointer changes to the crosshair shape, indicating Insert Mode. After placing each block or stream, you remain in Insert Mode until you click the Select Mode button in the upper right corner of the Model Library. For more information on what the mouse pointers mean, see Chapter 4.

Tip You can undock the Model Library and use it as a floating palette. You can also dock the Model Library under the toolbar.

For more details and examples for setting up a flowsheet, see *Getting Started, Building and Running a Process Model.*

The Data Browser

The Data Browser is a sheet and form viewer with a hierarchical tree view of the available simulation input, results, and objects that have been defined.

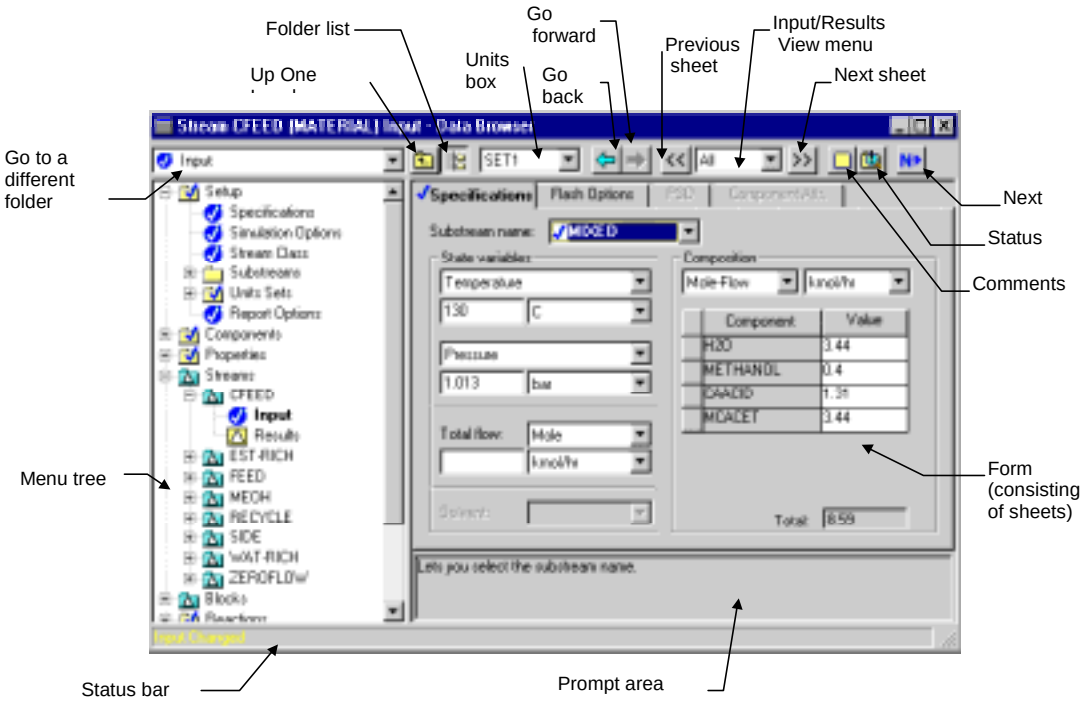
To open the Data Browser:

➤ Click the Data Browser button on the Data Browser toolbar.

– or –

➤ From the Data menu, click Data Browser.

The Data Browser also appears when you open any form.



Use the Data Browser to:

- Display forms and sheets and manipulate objects
- View multiple forms and sheets without returning to the Data menu, for example, when checking Properties Parameters input
- Edit the sheets that define the input for the flowsheet simulation
- Check the status and contents of a run
- See what results are available

The parts of the Data Browser window are:

Window Part	Description
Form	Displays sheets where you can enter data or view results
Menu Tree	Hierarchical tree of folders and forms
Status Bar	Displays status information about the current block, stream or other object
Prompt Area	Provides information to help you make choices or perform tasks
Go to a Different Folder	Enables you to select a folder or form to display.
Up One Level	Takes you up one level in the Menu Tree
Folder List	Displays or hides the Menu Tree
Units	Units of measure used for the active form
Go Back button	Takes you to the previously viewed form
Go Forward button	Takes you to the form where you last chose the Go Back Button
Input/Results View Menu	Allows you to view folders and forms for Input only, Results only, or All
Previous Sheet button	Takes you to the previous input or result sheet for this object
Next Sheet button	Takes you to the next input or result sheet for this object
Comments button	Allows you to enter comments for a particular block, stream, or other object
Status button	Displays any messages generated during the last run related to a particular form
Next button	Invokes the Aspen Plus expert system. Guides you through the steps required to complete your simulation.

Displaying Forms and Sheets in the Data Browser

Use the Data Browser to view and edit the forms and sheets that define the input and display the results for the flowsheet simulation. When you have a form displayed, you can view any sheet on the form by clicking on the tab for that sheet.

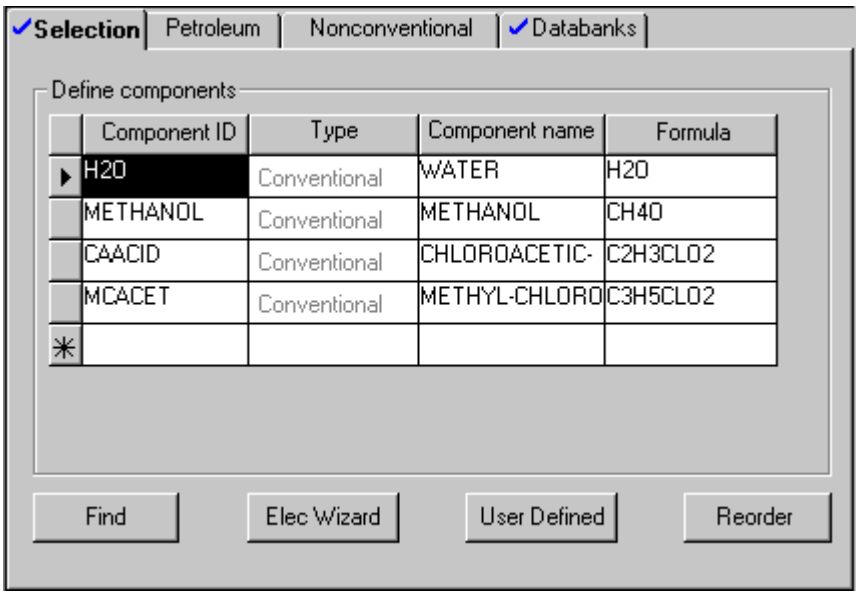
There are several ways to display forms. You can display a form in a new Data Browser by using:

- The Data menu
- Block or stream popup menus
- The Check Results button on the Control Panel, the Check Results command from the Run menu, or the Check Results button on the Simulation Run toolbar
- The Setup, Components, Properties, Streams, or Blocks buttons on the Data Browser toolbar
- The Next button on the Data Browser toolbar
- The Data Browser button on the Data Browser toolbar

You can move to a new form within the same data browser by using the:

- Menu tree
- Object Managers
- Next button on the Data Browser
- Previous Form and Next Form buttons (<<, >>)
- Go Back and Go Forward buttons (←, →)
- Select View menu
- Up One Level button

For example, the Components Specifications Selection form looks like this:



Note A form is a collection of sheets.

Status Indicators

Status indicators display the completion status for the entire simulation as well as for individual forms and sheets.

The status indicators appear:

- Next to sheet names on the tabs of a form
- As symbols representing forms in the Data Browser menu tree

This table shows the meaning of the symbols that appear:

This Symbol	On an	Means
	Input form	Required input complete
	Input form	Required input incomplete
	Input form	No data entered
	Mixed form	Input and Results
	Results form	No results present (calculations have not been run)
	Results form	Results available without Errors or Warnings (OK)
	Results form	Results available with Warnings
	Results form	Results available with Errors
	Results form	Results inconsistent with current input (input changed)
	Input folder	No data entered
	Input folder	Required input incomplete
	Input folder	Required input complete
	Results folder	No results present
	Results folder	Results available – OK
	Results folder	Results available with Warnings
	Results folder	Results available with Errors
	Results folder	Results inconsistent with current input (input changed)

Using Next

Click the Next button  to move to the next input form or menu at any point in Aspen Plus. The Next button is on the Data Browser toolbar in the main window and the toolbar of the Data Browser.

Use Next to:

- Guide you through the required and optional input for a run by displaying messages
- Tell you what you need to do next
- Ensure you do not make incomplete or inconsistent specifications, even when you change options and specifications you have already entered

This table shows what happens if you click Next:

If	Using Next
The sheet you are on is incomplete	Displays a message listing the input you must provide to complete the sheet.
The sheet you are on is complete	Takes you to next required input sheet for the current object.
You have selected an object that is complete	Takes you to next object or the next step in making a run.
You have selected an object that is incomplete	Takes you to the next sheet you must complete.

Using the Previous and Next Sheet Buttons

You can browse through sheets and forms sequentially by using the Previous Sheet and Next Sheet buttons on the Data Browser toolbar. These buttons take you through input sheets, results sheets, or both, depending on the current selection of the Input/Results View menu button in the Data Browser toolbar.

To view the next sheet in a series, click the Next Sheet button  .

To view the previous sheet, click the Previous Sheet button  .

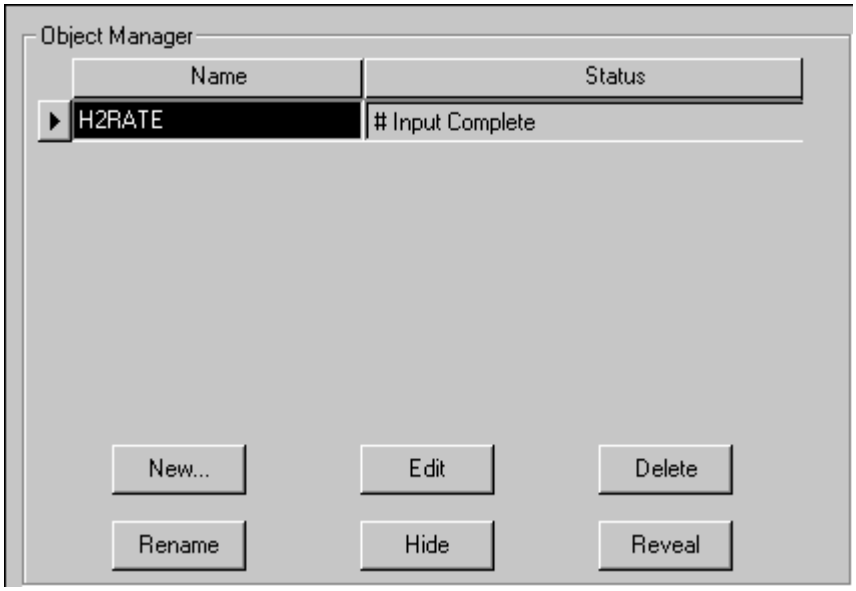
Using the Go Back and Go Forward Buttons

You can trace through previously viewed forms using the Go Back button  . The Go Back button can be clicked many times to continue through a reverse sequence of the forms you have viewed.

When you have gone back once, the Go Forward button  is enabled, so you can return to the form that you were on.

Using the Object Manager

Every block, stream, and other simulation object has a unique ID. When you select a folder in the Data Browser tree which contains several simulation objects, an Object Manager form appears in the form area of the Data Browser. For example:



Use the Object Manager buttons to perform the following functions:

Button	Description
New	Create a new object. You will be prompted for the ID for the object. The forms for the object will display.
Edit	Display the forms for the object
Delete	Delete the object
Clear	Delete the data for an object. The object still exists.
Rename	Rename the object
Hide	Temporarily remove an object from the simulation, without deleting it.
Reveal	Put a hidden object back into the simulation

Not all functions are available for all objects. For example, New is inactive on the Block Object Manager. Use the Process Flowsheet window and the Model Library to create a new block.

Deleting Objects and Clearing Forms

You can delete the following from a simulation:

- A component, from the Components Specification Selection sheet
- Blocks and streams, from the flowsheet
- Other input, such as a design specification, using the Data Browser or an Object Manager

When you delete input, all references to the deleted object (even on other forms) are automatically deleted. If this results in an inconsistent or incomplete specification, the Expert System marks the affected forms as incomplete, and the Next function takes you to any incomplete sheets.

You cannot delete:

- Sheets that do not represent objects, such as the Setup forms
- Properties Parameters (Binary or Pair) and Molecular Structure objects

However, you can clear these sheets of all existing input and restore their default values. To do this, click Clear from an Object Manager or from the menu that appears when you click the right mouse button on an item in the menu tree.

Using the Expert System When You Make Changes

The Aspen Plus Expert System (the Next function):

- Tells you when your specifications are inconsistent or incomplete
- Guides you through reconciling changes

If the field where you want to enter data is inactive, the Prompt for the field tells you why. To make the field active, delete any conflicting entries or options. For example, if you are using RadFrac to model a distillation column and specify None for the Reboiler, one of the Operating Specifications fields will become inactive since there is only one degree of freedom in the column specifications. If you change the Reboiler field, the other Operating Specification field will become active.

If you change an option or specification that makes other entries inconsistent, Aspen Plus displays a dialog box asking if you want to temporarily override the error.

Click Yes if you want to continue without correcting the inconsistency error. Then go to the affected fields and make them consistent with the new specification.

The affected forms are marked incomplete until you reconcile the specifications. The Expert System guides you to incomplete sheets.

Using Shortcut Keys

The following tables show the shortcut keys that are available in Aspen Plus.

- General shortcut keys
- Working with blocks and streams
- Editing
- Working with files
- Working with flowsheets
- Help
- Plotting
- Regions
- Running simulations
- Viewing

General Shortcut Keys

This table shows general shortcut keys:

Item	Shortcut Key
Close active window	ALT+F4
Copy	CTRL+C
Context Help	F1
Cut	CTRL+X
Display popup menu	SHIFT+F10
Display next MDI-child window	CTRL+F6
Paste	CTRL+V
Print	CTRL+P
Redo	CTRL+Y

Continued

Item	Shortcut Key
Save	CTRL+S
Select All	CTRL+A
Switch to next window	ALT+F6
What's This Help	SHIFT+F1

Shortcut Keys for Working with Blocks and Streams

This table shows the shortcut keys for working with blocks and streams:

Item	Shortcut Key
Align Blocks	CTRL+B
Center View	CTRL+HOME
Change Section	CTRL+F11
Change Stream Class	CTRL+Q
Delete Blocks or Streams	DEL
Exchange Icon	CTRL+K
Hide Annotation	CTRL+L
Hide Global Data	CTRL+G
Hide ID	CTRL+H
Input	CTRL+I
Rename Block or Stream	CTRL+M
Reroute Streams	CTRL+J
Results	CTRL+R
Stream Results	CTRL+D
Unplace Block or Group	CTRL+U

Shortcut Keys for Editing

This table shows the shortcut keys for editing:

Item	Shortcut Key
Copy	CTRL+C
Delete	DEL
Paste	CTRL+V
Rename	CTRL+M
Select All	CTRL+A

Shortcut Keys for Working with Files

This table shows the shortcut keys for working with files:

Item	Shortcut Key
Export	CTRL+E
Import	CTRL+T
New	CTRL+N
Open	CTRL+O
Print	CTRL+P
Save	CTRL+S

Shortcut Keys for Working with Flowsheets

This table shows the shortcut keys for working with flowsheets:

Item	Shortcut Key
Align Blocks	CTRL+B
Change Section	CTRL+F11
Change Stream Class	CTRL+Q

Continued

Item	Shortcut Key
Exchange Icons	CTRL+K
Flowsheet Sections	F11
Hide Annotation	CTRL+L
Hide Global Data	CTRL+G
Hide ID	CTRL+H
Reroute Streams	CTRL+J
Unplace Blocks	CTRL+U

Shortcut Keys for Help

This table shows the shortcut keys for help:

Item	Shortcut Key
Context Help	F1
Display popup menu	SHIFT+F10
What's This Help	SHIFT+F1

Shortcut Keys for Plotting

This table shows the shortcut keys for plotting:

Item	Shortcut Key
Display Plot	CTRL+ALT+P
Parametric Variable	CTRL+ALT+Z
Plot Wizard	CTRL+ALT+W
X-Axis Variable	CTRL+ALT+X
Y-Axis Variable	CTRL+ALT+Y

Shortcut Keys for Working with Regions

This table shows the shortcut keys for working with regions:

Item	Shortcut Key
Bookmarks	F3
Center View	CTRL+HOME
Page Break Preview	F2
Pan	CTRL+F3
Print	CTRL+P
Reset Page Breaks	SHIFT+F2
Select All	CTRL+A
Zoom Full	CTRL+END
Zoom In	CTRL+UP ARROW
Zoom Out	CTRL+DOWN ARROW

Shortcut Keys for Running Simulations

This table shows the shortcut keys that you can use when running simulations:

Item	Shortcut Key
Check Results	CTRL+F8
Connect to Engine	SHIFT+F7
Move To	CTRL+F9
Reinitialize	SHIFT+F5
Run	F5
Settings	CTRL+F7
Step	CTRL+F5
Stop Points	F9

Shortcut Keys for Viewing

This table shows the shortcut keys that you can use for viewing:

Item	Shortcut Key
Annotation	CTRL+ALT+L
Bookmarks	F3
Center View	CTRL+HOME
Control Panel	F6
Current Section Only	SHIFT+F11
Global Data	CTRL+ALT+G
History	CTRL+ALT+H
Input Summary	CTRL+ALT+I
OLE Objects	CTRL+ALT+F
Model Library	F10
Page Break Preview	F2
Pan	CTRL+F3
PFD Mode	F12
Redraw	CTRL+W
Refresh PFD	SHIFT+F12
Report	CTRL+ALT+R
Reset Page Breaks	SHIFT+F2
Zoom Full	CTRL+END
Zoom In	CTRL+UP ARROW
Zoom Out	CTRL+DOWN ARROW

Supplying Comments

You can write notes or keep track of information by entering comments for particular forms. Each object has just one Comments form which you can access from any input or results form for the object.

To enter comments on a form:

1. Click the Comments button on the Data Browser toolbar.

   If there are no existing comments, the button looks like this:  .

   If there are existing comments, the button looks like this: 

2. Enter your one line description in the Description box of the Comments form.

   The description is printed in the Aspen Plus report.

3. Enter your comments in the Comments area of the Comments form.
4. Click OK to close the Comments form.

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2 Creating a Simulation Model

This chapter describes how to use Aspen Plus to create a simulation model, including the following topics:

- Creating a new run
- Selecting a Template
- Selecting a Run Type
- Completing the input specifications for a run
- About the templates
- The Aspen Plus online applications library

Process Simulation Using Aspen Plus

Process simulation with Aspen Plus allows you to predict the behavior of a process using basic engineering relationships such as mass and energy balances, phase and chemical equilibrium, and reaction kinetics. Given reliable thermodynamic data, realistic operating conditions, and the rigorous Aspen Plus equipment models, you can simulate actual plant behavior. Aspen Plus can help you design better plants and increase profitability in existing plants.

With Aspen Plus you can interactively change specifications, such as flowsheet configuration, operating conditions, and feed compositions, to run new cases and analyze alternatives. To analyze your results, you can generate plots, reports, PFD-style drawings, and spreadsheet files.

Aspen Plus allows you to perform a wide range of additional tasks. You can:

- Perform sensitivity analyses and case studies
- Generate custom graphical and tabular output
- Estimate and regress physical properties
- Fit simulation models to plant data
- Optimize your process
- Interface results to spreadsheets
- Share input and results among other Windows applications using OLE

Aspen Plus contains data, properties, unit operation models, built-in defaults, reports, and other features and capabilities developed for specific industrial applications, such as petroleum simulation. For more information about industry-specific defaults and features, see Selecting a Template on page 2-3.

Creating a New Run

Follow these instructions to either:

- Start Aspen Plus and create a new run
- Create a new run when you are already in Aspen Plus

Starting Aspen Plus and Creating a New Run

To start Aspen Plus and create a new run:

1. Start Aspen Plus from the Start Menu or by double-clicking the Aspen Plus icon on your desktop.
2. On the Aspen Plus Startup dialog box, click the appropriate button to create a new simulation using a Blank Simulation or a Template, then click OK.
3. If you choose a blank simulation, the Aspen Plus main window opens and you can begin building your new model.
4. If you choose a Template, follow the steps below.
5. In the New dialog box, select the type of simulation template and the units you wish to use, from the list. For more information on choosing a Template, see Selecting a Template on page 2-3.
6. Choose the desired Run Type in the Run Type list box. For more information, see Selecting a Run Type on page 2-4.
7. Click OK.

8. If the Connect to Engine dialog box appears, specify where the Aspen Plus engine will execute. See Chapter 1 for more information.

Creating a New Run in Aspen Plus

To create a new run if you are already in Aspen Plus:

1. Save the current run if you want to open it later.
2. From the File menu, click New.
3. A dialog box appears, asking if you want to close the current run before opening a new run. Click Yes, No, or Cancel:

If you choose	This happens
Yes	The current run will be closed, and the new run will open in the existing Aspen Plus window. You will be given the option to save the current run before the new run opens.
No	The current run will remain active in the existing window, and a new run will open in a second Aspen Plus window.
Cancel	You will be returned to the current run.

4. In the New dialog box, select the type of simulation Template and the units you wish to use, from the list. For more information on choosing a Template, see Selecting a Template on page 2-3.
5. Choose the desired Run Type in the Run Type list box. For more information on Run Types, see Selecting a Run Type on page 2-4.
6. Click OK.

Selecting a Template

When starting a new simulation, you can start with a blank simulation or you can begin with a Template. Templates set defaults commonly used by specific industries for:

- Units of measurement
- Stream composition information and properties to report
- Stream report format
- Default setting for Free-Water option
- Property method

- Other application-specific defaults

For information about creating your own templates, see Chapter 16.

There are built-in Templates for the following applications:

- Air Separation
- Chemicals
- Electrolytes
- Gas Processing
- General
- Hydrometallurgy
- Petroleum
- Pharmaceuticals
- Pyrometallurgy
- Solids
- Specialty Chemicals

For each Template, you can select either metric or English units of measurement as a default units set. Other units sets are also available.

See the sections at the end of this chapter for a description of the Templates.

Selecting a Run Type

When creating a new run, you must select a Run Type from the Run Type list box on the New dialog box.

Use the Flowsheet run type for flowsheet simulations (including sensitivity studies and optimization). Flowsheet runs can also include the following calculations integrated with a flowsheet simulation:

- Property constant estimation
- Assay data analysis/pseudocomponents generation
- Property analysis

Other run types are used to run Aspen Plus without performing a flowsheet simulation:

Run Type	Description	Use to
Assay Data Analysis	A standalone assay data analysis/pseudocomponents generation run	Analyze assay data when you do not want to perform a flowsheet simulation in the same run. See Chapter 32.
Data Regression	A standalone data regression run. Can contain property constant estimation and property analysis calculations.	Fit physical property model parameters required by Aspen Plus to measured pure component, VLE, LLE and other mixture data. Aspen Plus cannot perform data regression in a Flowsheet run. See Chapter 31.
PROPERTIES PLUS	A PROPERTIES PLUS setup run	Prepare a property package for use with Aspen Custom Modeler or ADVENT, with third-party commercial engineering programs, or with your company's in-house programs. You must be licensed to use PROPERTIES PLUS.
Property Analysis	A standalone property analysis run. Can contain property constant estimation and assay data analysis calculations.	Perform property analysis by generating tables of physical property values when you do not want to perform a flowsheet simulation in the same run. See Chapter 29.
Property Estimation	A standalone property constant estimation run	Estimate property parameters when you do not want to perform a flowsheet simulation in the same run. See Chapter 30.

Completing Input Specifications for a Run

For Flowsheet runs, follow these basic steps to complete the required and optional input specifications:

1. Define the simulation flowsheet (blocks, streams, and connectivity) in the Process Flowsheet window. See Chapter 4.

2. Enter required input specifications on the following forms in the Data Browser:

Forms	Specify
Setup	Global simulation options (see Chapter 5)
Components	Conventional chemical components, petroleum assays, and pseudocomponents in the simulation. For information on working with components, see Chapter 6. For more information on petroleum assays and pseudocomponents, see Chapter 32.
Physical Properties	Methods and data to use for calculating physical properties. For more information on entering property methods and entering property parameters and data, see Chapters 7 and 8 respectively.
Streams	Feed stream compositions, flows, and conditions. For more information, on specifying streams, see Chapter 9.
Blocks	Design and operating conditions for each unit operation block in the flowsheet (see Chapter 10).

3. Provide additional specifications if needed by opening the Data Browser and using the forms shown in this table:

Use these forms	To
Reactions	Define electrolytes chemistry; specify reaction kinetics for use in reactor and reactive distillation models (see Chapter 27)
Convergence	Specify automatic flowsheet analysis options; specify user-defined tear streams, convergence blocks, and sequences (see Chapter 17)
Flowsheeting Options	Add additional constraints and specifications to the flowsheet model. Request pressure relief calculations
Model Analysis Tools	Specify sensitivity studies, optimization runs, and Data-Fit problems. Data-Fit is used to fit simulation models to plant or laboratory data.
Setup ReportOptions	Specify options for generating the Aspen Plus report. For more information on specifying the elements in the Report file and on generating the report file, see Chapters 5 and 12 respectively.

Tip Although you can enter most specifications in any order, it is best to use Next and let the Aspen Plus Expert System guide you. For more information on using Next see Chapter 1.

Completion Status for the Flowsheet

The completion status for the overall flowsheet appears in the status bar of the main window. When completing specifications for a run, you see the following status messages:

This status message	Means	You can
Flowsheet Not Complete	The simulation flowsheet has not been defined or the flowsheet connectivity is incomplete.	Use Next on the Data Browser toolbar to find out why connectivity is incomplete.
Required Input Incomplete	Input specifications for the run are incomplete.	Use Next from the main window or Data Browser toolbars to find out what you must specify to complete the input specifications and to go to forms that are incomplete.
Required Input Complete	Required input specifications for the run are complete.	Run the simulation or enter optional specifications.

Completion Status on Forms

The completion status for the active form or menu appears in the status bar of the Data Browser. When completing specifications for a new run, you see the following status messages:

This status message	Means	You can
Required Input Incomplete	Input specifications for the form or object are incomplete.	Use Next from the Data Browser toolbar to find out what you must specify to complete the input specifications.
Input Complete	Required input specifications for the form or object are complete.	Enter specifications for other forms or run the simulation.

Completion Status Indicators in the Data Browser Menu Tree

In the Data Browser menu tree, the following symbols indicate the input completion status:

Symbol	In an	Means
	Input form	Required Input Complete
	Input form	Required Input Incomplete
	Input form	No data entered
	Mixed form	Input and Results
	Results form	No results present (calculations have not been run)
	Results form	Results available without Errors or Warnings (OK)
	Results form	Results available with Warnings
	Results form	Results available with Errors
	Results form	Results inconsistent with current input (input changed)
	Input folder	No data
	Input folder	Input Incomplete
	Input folder	Input complete
	Results folder	No results present
	Results folder	Results available without Errors or Warnings (OK)
	Results folder	Results available with Warnings
	Results folder	Results available with Errors
	Results folder	Results inconsistent with current input (input changed)

Completion Status Indicators on Sheets

On forms, the completion status for each individual sheet is displayed on the sheet tab:

Symbol	Means
	Input specifications for the sheet are incomplete. Click the tab of the incomplete sheet and complete the input – or – Use Next
	Input specifications for the sheet are complete. The required input has been entered by the user.
(blank)	Input for this sheet is optional.

Completion Status for Objects

When you are on an Object Manager for a block or other object, the completion status for each object appears in the Status column.

Status message	Means	You can
Input Incomplete	Input specifications for the object are incomplete.	Use Next from the Data Browser toolbar to go to an incomplete form, or select an incomplete object from the Object Manager, and click Edit.
Input Complete	Required input specifications for the object are complete.	Use Next from the Data Browser toolbar to go to the next step, or enter optional specifications by selecting an object from the Object Manager and clicking Edit.
Results Present	Results are present.	View results, make input changes, and re-run the simulation
Input Changed	Results are present, the input specifications have been changed and the input is complete.	View results, make further input changes, and re-run the simulation

About the Templates

There are built-in Templates for the following applications:

- Air Separation
- Chemicals

- Electrolytes
- Gas Processing
- General
- Hydrometallurgy
- Petroleum
- Pharmaceuticals
- Pyrometallurgy
- Solids
- Specialty Chemicals

About the General Template

Use the General Template for a wide range of vapor-liquid applications. The General Template defines the following units sets. These units sets are also available in all other Templates. For more information on units sets, see Chapter 5.

Unit-Set	Temp	Pres	Mass Flow	Mole Flow	Enthalpy Flow	Volume Flow
ENG†	F	psi	lb/hr	lbmol/hr	Btu/hr	cuft/hr
MET	K	atm	kg/hr	kmol/hr	cal/sec	l/min
METCBAR††	C	bar	kg/hr	kmol/hr	MMkcal/hr	cum/hr
METCKGGM	C	kg/sqcm	kg/hr	kmol/hr	MMkcal/hr	cum/hr
SI	K	n/sqm	kg/sec	kmol/sec	watt	cum/sec
SI-CBAR	C	bar	kg/hr	kmol/hr	watt	cum/hr

† *Default English units set for General Template*

†† *Default metric units set for General Template*

General Template Defaults

The General Template sets the following defaults. See Chapter 5 for information about setting and changing defaults.

Specification	Default
Physical property method	None
Flow-basis for input	Mole
Stream report composition	Mole flow
Stream report format	General purpose with enthalpy and density on a mass basis. Entropy is not reported.
Stream class	Conventional. Appropriate for systems containing vapor, liquid, and salts.

General Template Property Sets

The General Template defines the following property sets. These property sets are also available in many of the other Templates. For more information about property sets, see Chapter 28.

Property Set	Description
HXDESIGN	Thermal and transport properties in SI units needed by heat exchanger design programs and ADVENT, including:
	Mass vapor fraction
	Mass flow rate for total, vapor, and liquid phases
	Mass enthalpy for total, vapor, and liquid phases
	Mass density for total, vapor, and liquid phases
	Mass heat capacity for total, vapor, and liquid phases
	Pseudo-critical pressure for total, vapor, and liquid phases:
	Viscosity for vapor and liquid phases
	Thermal conductivity for vapor and liquid phases
	Average molecular weight for total, vapor, and liquid phases
THERMAL	Thermal properties, including:
	Vapor and liquid phase enthalpy
	Vapor and liquid phase heat capacity
	Vapor and liquid phase thermal conductivity

Continued

Property	Description
TXPORT	Transport properties, including:
	Vapor and liquid phase mass density
	Vapor and liquid phase viscosity
	Liquid phase surface tension
VLE	Vapor-liquid equilibrium component information, including:
	Component fugacity coefficient in vapor and liquid phases
	Component activity coefficient in liquid phase
	Pure component vapor pressure
VLLE	Vapor-liquid-liquid equilibrium component information, including:
	Component fugacity coefficient in each phase
	Component activity coefficient in each liquid phase
	Pure component vapor pressure

About the Petroleum Template

The Petroleum Template defines defaults commonly used in the petroleum industry. It is also appropriate for petrochemical applications such as ethylene plants, which involve petroleum fractions as feedstocks.

This table shows the defaults used:

Specification	English Default	Metric Default
Units	F, psi, lb/hr, lbmol/hr, MMBtu/hr, bbl/day	C, bar, kg/hr, kmol/hr, MMkcal/hr, bbl/day
Physical property method	None	None
Free water	Yes (see Chapter 5)	Yes (see Chapter 5)
Flow basis	Standard liquid volume	Mass
Stream report composition	Standard liquid volume flow	Mass flow

Because petroleum applications encompass a wide range of boiling fractions/components and process conditions, this Template does not have a default physical property method. These methods are used most frequently:

- BK10
- CHAO-SEA
- GRAYSON
- RK-SOAVE

- PENG-ROB
- IDEAL

You should consider additional methods for various operations within a refinery (such as ELECNRTL for sour water strippers and amine treatment units, and UNIFAC for aromatic extraction). For information to help you determine which property method is best for your application, see Chapter 7.

Aspen Plus provides comprehensive methods for analyzing assay data and automatically generating pseudocomponents. You can select from five built-in pseudocomponent property methods to characterize pseudocomponents. You can also enter curves of petroleum properties, such as sulfur and metal contents. Aspen Plus tracks these properties throughout the flowsheet. You can use them in design specifications, optimization constraints, and objective functions. See Chapter 32 for more information.

The Aspen Plus PetroFrac model simulates a wide range of fractionation units within a refinery. PetroFrac can model a tower with any number of:

- Side strippers, including the bottom liquid return to the main tower
- Pumparounds and bypasses
- Partial and total drawoffs

PetroFrac can model the feed furnace as an integral part of the tower, including the slop cut recycle for a vacuum unit. It lets you enter petroleum-specific property specifications, such as ASTM distillation temperatures, gaps, and overlaps. It also offers extensive column sizing and rating capabilities, including the ability to handle structured packings and integrated pressure drop calculations. For complete information on PetroFrac, see the *Aspen Plus Unit Operation Models manual*.

Petroleum Property Sets

In Aspen Plus, many properties can be used to characterize streams in a refinery. Chapter 28 lists these properties and explains how to use them.

The Petroleum Template includes property sets for many widely used petroleum-related properties.

Property Set	Description
CUTS-E	Standard liquid volume flow of petroleum cuts at 100º F intervals. Valuable for concise reporting of stream composition.
CUTS-M	Mass flow rate of petroleum cuts at 50º C intervals. Valuable for concise reporting of stream composition.
D86-5	ASTM D86 temperature at 5 liquid volume %
D86-95	ASTM D86 temperature at 95 liquid volume %

Continued

Property Set	Description
GASPROPS	Vapor phase properties, including:
	Compressibility factor for a mixture
	Actual volume flow
	Standard vapor volume flow
	Heat capacity ratio (CP/CV)
KINVISC	Kinematic viscosity at 100°F and 212°F or 40°C and 100°C (dry basis)
LIGHT	Petroleum characteristics for light distillates (dry basis), including:
	Reid vapor pressure
	Flash point based on API method
	Aniline point
MIDDLE	Petroleum characteristics for middle distillates (dry basis), including:
	Cetane number
	Flash point based on API method
	Pour point based on API method
	Aniline point
PETRO†	General petroleum properties on dry basis, including:
	Standard liquid volume flow (bbl/day) and (bbl/hr)
	Standard API gravity
	Standard specific gravity
	Watson UOP K-factor
	True boiling point distillation curve
	ASTM D86 distillation curve
	ASTM D1160 distillation curve
TBP-5	True boiling point temperature at 5 liquid volume %
TBP-95	True boiling point temperature at 95 liquid volume %

† *Default for stream results*

Petroleum Stream Report Options

The large number of pseudocomponents and distillation curves in a petroleum application can result in a lengthy stream report.

The Petroleum Template defines several stream report format (TFF) options so you can view or print subsets of stream information:

TFF	Displays
PETRO-E	State variables, stream flows, properties, distillation curves, component flows. Standard volume flows of the 100°F petroleum cuts if CUTS-E property set was selected
PETRO-M	State variables, stream flows, properties, distillation curves, component flows. Mass flows of the 50°C petroleum cuts if CUTS-M property set was selected
PET-COMP	Only component flow and total flow results
PET-CURVE	Only distillation curve stream results
PET-PROP	Only state variables, stream flows, properties, and flows of petroleum cuts

About the Gas Processing Template

The Gas Processing Template defines defaults commonly used in the gas processing industry. For example, stream flows are standard vapor volume flows in millions of standard cubic feet per day or millions of standard cubic meters per hour.

The gas processing defaults are:

Specification	Default
English units	F, psi, lb/hr, MMscfd, MMbtu/hr, MMcuft/hr
Metric units	C, bar, tonne/hr, MMscmh, MMkcal/hr, cum/hr
Physical property method	Peng-Robinson
Flow basis	Mole with MMscfd† or MMscmh††
Stream report compositions	Mole flow with MMscfd† or MMscmh††

† *MMscfd is millions of standard cubic feet per day.*

†† *MMscmh is millions of standard cubic meters per hour.*

Peng-Robinson is the default method for calculating physical properties. For many gas processing applications, such as gas sweetening, gas dehydration, and the Claus process, you may want to select other physical property methods. For help selecting physical property methods for your application, see Chapter 7. For example, you may want to use the ELECNRTL method together with the special amines data package for gas sweetening.

Gas Processing Property Sets

This Template also provides property sets commonly needed in gas processing applications:

Property Set	Description
CRITICAL	Pseudo critical properties, including:
	Pseudo critical temperature
	Pseudo critical pressure
	Pseudo critical volume
GASPROPS†	General gas properties, including:
	Compressibility factor
	Actual volume flow
	Standard vapor volume (MMscfd†† or MMscmh†††)
	Heat Capacity Ratio (CP/CV) for mixture
TDEW	Dew point temperature

† *Default for stream results*

†† *MMSCFD is millions of standard cubic feet per day.*

††† *MMSCMH is millions of standard cubic meters per hour.*

About the Air Separation Template

Use the Air Separation Template for cryogenic air separation simulations. The defaults are:

Specification	Default
English units	F, psi, lb/hr, lbmol/hr, Btu/hr, cuft/hr
Metric units	C, bar, kg/hr, kmol/hr, watt, cum/hr
Physical property method	Peng-Robinson
Components included	O2, N2, AR
Flow basis	Mole
Stream report composition	Mole flow and mole fraction

These Aspen Plus unit operation models are used extensively in air separation simulations:

Model	Description
RadFrac	Rigorous distillation
MultiFrac	Multiple column simulation
HeatX	Rigorous heat exchange
MHeatX	Cold box heat exchange

The MultiFrac model is especially useful for modeling the double- and triple-column systems typically found in air plants. MultiFrac solves these interlinked column systems as a single unit, without recycle flow estimates.

Air plants are highly heat-integrated. You can specify heat streams to model the complex heat integration between units.

Air Separation Property Sets

The air separation property sets are:

Property Set	Description
CRITICAL	Pseudo critical properties, including:
	Pseudo critical temperature
	Pseudo critical pressure
	Pseudo critical volume
GASPROPS†	General gas properties, including:
	Compressibility factor
	Actual volume flow
	Standard vapor volume (MMscfd†† or MMscmh†††)
	Heat Capacity Ratio (CP/CV) for mixture
TBUBBLE	Bubble point temperature
TDEW	Dew point temperature

† *Default for stream results*

†† *MMscfd is millions of standard cubic feet per day.*

††† *MMSCMH is millions of standard cubic meters per hour.*

About the Chemicals Template

The Chemicals Template is suitable for a wide range of chemical (non-electrolyte) applications. It is also appropriate for petrochemical applications, such as MTBE production and VCM plants, where feedstocks are defined in terms of chemical components.

The defaults are:

Specification	Default
English units	F, psi, lb/hr, lbmol/hr, Btu/hr, cuft/hr
Metric units	C, bar, kg/hr, kmol/hr, MMkcal/hr, cum/hr
Physical property method	NRTL
Flow basis	Mole
Stream report composition	Mole flow

The default base property method is NRTL, which has wide application for low-pressure ideal and non-ideal chemical systems. Aspen Plus has several additional activity coefficient models and equations of state for modeling chemical systems. For example, for systems containing organic acids, use NRTL-HOC, WILS-HOC, or UNIQ-HOC methods. For chemical systems at high pressures, use an equation-of-state method, such as RK-ASPEN, SR-POLAR, PRWS, PRMHV2, or PSRK. For more information on Aspen Plus physical property methods, see Chapter 7.

Each activity coefficient and equation-of-state model has a large databank of binary interaction parameters suitable for modeling chemical systems. Aspen Plus automatically retrieves and displays these binary parameters. If the database does not have binary parameters for a component pair, Aspen Plus can estimate the missing binary parameters for your application (see Chapter 30).

If you have measured data for your chemical system you can use Aspen Plus to regress model parameters. For more information on regressing property data, see Chapter 31. Aspen Plus has interactive tools for analyzing the properties and vapor-liquid equilibrium of chemical systems. For more information on property analysis, see Chapter 29.

The built-in property sets are the same as for the General Template.

About the Electrolytes Template

The Electrolytes Template is used for applications that require rigorous modeling of electrolyte species. You can use this Template in any application where electrolytes are important.

The defaults are:

Specification	Default
English units	F, psi, lb/hr, lbmol/hr, Btu/hr, cuft/hr
Metric units	C, bar, kg/hr, kmol/hr, MMkcal/hr, cum/hr
Physical property method	ELECNRTL
Components included	H2O
Flow basis	Mass
Stream report composition	Mass flow
Stream report format	Displays all electrolyte properties that are requested in property sets

The ELECNRTL property method model is recommended for rigorously modeling electrolyte systems. This property method is described in more detail in Chapter 7.

Aspen Plus has a large built-in databank of electrolyte reactions and interaction parameters for many electrolyte systems. The Aspen Plus Electrolytes Wizard generates electrolytes chemistry automatically and interactively, so you can control the species and reactions to include in your simulation. See Chapter 6 and Aspen Plus Getting Started Modeling Processes with Electrolytes for instructions on how to build an electrolytes application.

Electrolytes Property Sets

The built-in property sets are:

Property Set	Property Description
FAPP	Apparent component mole flow
FTRUE	True component mole flow
LVOLFLOW	Liquid volumetric flow
MASSCONC	Mass concentration
MOLECONC	Mole concentration
PH	pH at current temperature

Continued

Property Set	Property Description
SOLINDEX	Solubility index
TBUBBLE	Bubble point temperature
VMOLFLOW	Component mole flows in vapor phase
VMOLFRAC	Component mole fractions in vapor phase
WXAPP	Apparent component mass fraction
WAPP	Apparent component mass flow
XTRUE	True component mole fraction

About the Specialty Chemicals Template

The Specialty Chemicals Template is for specialty chemical applications, with or without electrolytes. You can view stream results on a:

- Concentration basis
- Per batch basis, if you select the Batch-Operations report option (see Chapter 12)

The defaults for this Template are:

Specification	Default
English units	F, psi, lb/hr, lbmol/hr, Btu/hr, gal/hr
Metric units	C, bar, kg/hr, kmol/hr, kcal/hr, l/hr
Physical property method	NRTL
Flow basis	Mass
Stream report composition	Mass flow
Stream report format	Displays standard properties, plus concentration and batch stream report, if requested. Electrolyte properties are also displayed if an electrolyte method and electrolyte property set are selected.

Aspen Plus has two batch unit operation models that are especially useful for specialty chemicals applications:

- RBatch, a batch reactor
- BatchFrac, for batch distillation

See Chapter 10 or *Aspen Plus Unit Operation Models* for more information.

The default base property method is NRTL, which has wide application for low-pressure ideal and non-ideal chemical systems. Aspen Plus has additional activity coefficient models and equations of state for modeling chemical systems. For more information on Aspen Plus physical property methods, see Chapter 7.

Each activity coefficient model has a large databank of binary interaction parameters suitable for modeling chemical systems. Aspen Plus automatically retrieves and displays these binary parameters. If the database does not have binary parameters for a component pair, Aspen Plus can estimate the missing binary parameters for your application.

If you have measured data for your chemical system, you can use Aspen Plus to regress model parameters. Aspen Plus has interactive tools for analyzing the properties and vapor-liquid equilibrium of chemical systems. For more information on property analysis, see Chapter 29.

If your process involves electrolytes, use the Electrolytes Wizard to define the reactions and ionic species. For more information on the Electrolytes Wizard, see Chapter 6. The NRTL method will be replaced by ELECNRTL, and the electrolytes database will be used.

The built-in property sets are the same as for the Electrolytes Template.

About the Pharmaceuticals Template

The Pharmaceuticals Template uses NRTL as the default base property method. You can use this method for two-liquid-phase systems, or vapor and liquid systems at low pressure. This Template reports stream composition on a mass concentration and mass flow basis. You can also view the vapor-liquid-liquid equilibrium for any stream and examine results on a per batch basis, if you select the Batch-Operations report option.

The defaults for this Template are:

Specification	Default
English units	F, psi, lb/hr, lbmol/hr, Btu/hr, gal/hr
Metric units	C, bar, kg/hr, kmol/hr, kcal/hr, l/hr
Physical property method	NRTL
Flow basis	Mass
Stream report composition	Mass flow and mass concentration
Stream report format	Displays standard properties, plus batch stream report if requested

Aspen Plus has two batch unit operation models that are especially useful for pharmaceutical applications:

- RBatch, a batch reactor
- BatchFrac, for batch distillation

For more information, see Chapter 10 or Aspen Plus Unit Operation Models.

The built-in property sets are:

Property Set	Description
LVOLFLOW	Liquid volumetric flow
MASSCONC†	Mass concentration
MOLECONC	Mole concentration
VMOLFLOW	Component mole flows in vapor phase
VMOLFRAC	Component mole fractions in vapor phase

† *Default for stream report*

About the Hydrometallurgy Template

Use the Hydrometallurgy Template to model electrolytes and solids in hydrometallurgical processes.

The defaults for this Template are:

Specification	Default
English units	F, psi, lb/hr, lbmol/hr, Btu/HR, cuft/hr
Metric units	C, bar, kg/hr, kmol/hr, MMkcal/HR, cum/hr
Physical property method	ELECNRTL
Component included	H2O
Flow basis	Mass
Stream class	MIXCISLD, for modeling hydrometallurgy systems with vapor, liquid, electrolytes, salts, and inert molecular solids.
Stream report composition	Not displayed with default stream report format
Stream report format	Displays all substreams together

The ELECNRTL property method is recommended for rigorously modeling the electrolyte systems present in hydrometallurgy processes. This property method is described in more detail in Chapter 7 and in Aspen Plus Physical Property Methods and Models, Chapter 2.

Aspen Plus has a large built-in databank of electrolyte reactions and interaction parameters for many electrolyte systems. The Aspen Plus Electrolytes Wizard generates electrolytes chemistry automatically and interactively, so you can control the species and reactions to include in your simulation. See Chapter 6 and *Aspen Plus Getting Started Modeling Processes with Electrolytes* for instructions on how to build an electrolytes application.

Property Sets for Hydrometallurgy

The built-in property sets for hydrometallurgical simulations include all property sets listed for Electrolytes Simulation, plus the following:

Property Set	Description
ALL-SUBS	Characteristics for entire stream, including:
	Temperature
	Pressure
	Volumetric flow
	Mass vapor fraction
	Mass solids fraction
	Mass density
	Mass flow
	This property set is the default for stream report

About the Pyrometallurgy Template

Use the Pyrometallurgy Template to model high temperature metals processing applications. The defaults are:

Specification	Default
English units	F, psi, lb/hr, lbmol/hr, Btu/hr, cuft/hr
Metric units	C, bar, tonne/hr, kmol/hr, MMkcal/hr, cum/hr
Physical property method	SOLIDS
Flow basis	Mass
Stream class	MIXCISLD, for modeling pyrometallurgy systems with only molecular species. If you have ores that must be defined as non-conventional components or if you need to model particle size distribution, you will need a different stream class (see Chapter 9).
Stream report composition	Not displayed with default stream report format
Stream report format	Displays all substreams together

Pyrometallurgical processes often involve chemical and phase equilibrium between multiple liquid phases and a vapor phase. Aspen Plus uses the RGibbs model to simulate these multiphase operations. Pyrometallurgical applications often require different activity coefficient models for different liquid phases in the system. You can create multiple methods, based on the SOLIDS method, to use different activity coefficient models. You can then assign the new method to specified liquid phases. For more details on how to modify a physical property method, see Chapter 7.

Pyrometallurgy Property Sets

The pyrometallurgy property sets are:

Property Set	Description
ALL-SUBS†	Characteristics for entire stream, including:
	Temperature
	Pressure
	Volumetric flow
	Mass vapor fraction
	Mass solids fraction
	Mass density
	Mass flow
VMOLFLOW	Vapor mole flow
VMOLFRAC	Vapor component mole fractions

†*Default for stream results*

About the Solids Template

Aspen Plus can model solids anywhere in a process flowsheet. A wide range of unit operation models for solids handling equipment is available, including crystallizers, crushers, screens, and cyclones. See Aspen Plus Unit Operation Models for more information on the models. See Getting Started Modeling Processes with Solids to learn how to model solids processes step-by-step.

The Solids Template reports the properties and component flows of all types of components (vapor, liquid, and solid) together. You can also request Aspen Plus to report:

- Overall stream concentrations
- Vapor fractions
- Solid fractions

If you use attributes in your simulation, substream and component attributes appear in the default stream report.

The defaults for this Template are:

Specification	Default
English units	F, psi, lb/hr, lbmol/hr, Btu/hr, cuft/hr
Metric units	C, bar, kg/hr, kmol/hr, MMkcal/hr, cum/hr
Physical property method	None, but SOLIDS is recommended
Flow basis	Mass
Stream class	MIXCISLD, but you will often want to select a different stream class based on your application
Stream report composition	Not displayed with default stream report format
Stream report format	Displays all substreams together

Solids Property Sets

The built-in property sets for solids are:

Property Set	Description
ALL-SUBS†	Characteristics for entire stream, including: Temperature Pressure Volumetric flow Mass vapor fraction Mass solids fraction Mass density Mass flow
MASSCONC	Mass concentration
MOLECONC	Mole concentration
VMOLFLOW	Component mole flows in vapor phase
VMOLFRAC	Component mole fractions in vapor phase

† *Default for stream results*

Using the Online Applications Library

Aspen Plus includes a library of Application Examples to illustrate how Aspen Plus is used to solve a range of industrial problems.

These application examples cover a range of process industries, including gas processing, petroleum refining, petrochemicals, chemicals, pharmaceuticals, and metals processing. You can examine the input and results for these applications, see how to use various Aspen Plus features, and modify and run these applications to simulate your own processes.

These examples demonstrate the value of many Aspen Plus features, including residue curves, three-phase reactive distillation, rigorous heat exchange rating, and extraction with user liquid-liquid distribution correlations.

Accessing the Online Applications Library

To access the online applications library in Aspen Plus:

1. From the File menu, click Open.

   – or –

   If you have just started Aspen Plus, from the Aspen Plus Startup dialog box, click Open an Existing Simulation, select More Files… from the list of files, and Click OK.

2. In the Open dialog box, click the Favorites button  .
3. Click the app directory.
4. To view a description of a file, click the file then click the Preview button  on the Open dialog box toolbar.
5. Click the file you want to open, then click Open.
6. The input and results are then loaded. You can examine, modify, and run the simulation.

Examining Descriptions of Files

To view a description of a file before opening it:

➤ Click the file then click the Preview button (button that is furthest right) on the Open dialog box toolbar.

To view a description of an open file:

1. From the Data menu, click Setup, then click Specifications.
2. Click the Description sheet.

To examine available comments for blocks and other objects, click the Comments button from the toolbar of the Data Browser.

If comments are available, the Comments button looks like this: 

If there are no comments available, the Comments button looks like this: 

❖ ❖ ❖ ❖

3 Using Aspen Plus Help

Aspen Plus has online Help, prompts and expert system messages, to give you information as you use the program.

This chapter explains how to use Help including:

- Getting online Help
- Using hypertext links
- Using the Back button
- Searching for help on a topic
- Printing help

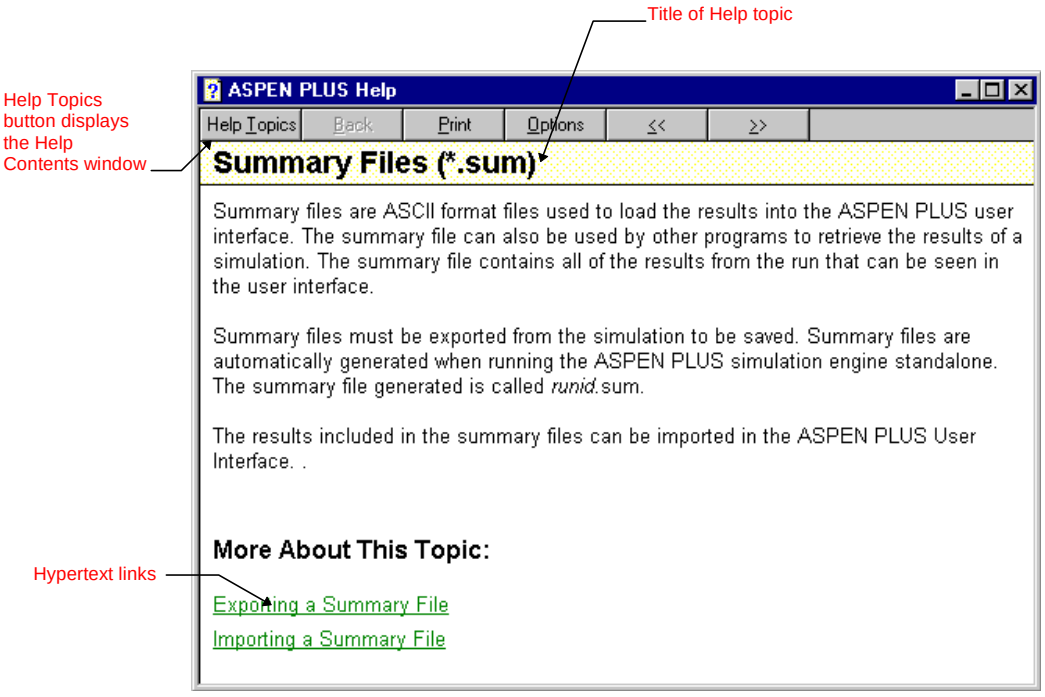
Getting Help

There are several ways to get help in Aspen Plus:

If you want help about	Do this
A particular topic	On the Help menu, click Help Topics. From the Help Topics dialog box, click the Index tab.
A form or field	On the Aspen Plus toolbar, click the What's This button then click the field or form.
A dialog box	Click the Help button on the dialog box.
The item the cursor or mouse pointer is on	Press F1.

About The Help Window

Aspen Plus help topics appear in Help windows.



This table provides more information about elements you might find on a Help window:

Window Element	Description
Help title	Title of the help topic currently displayed in the Help window. For example, Aspen Plus Help.
Hyperlink	A word or phrase that displays information on a related topic when you click it
See Also hyperlink	An additional topic you can move to by clicking it
Help Topics button or Contents button	Displays the Help Contents window, including Contents, Index and Find tabs
Back button	Returns you to the last help topic you viewed
Search button	Displays the Index. You can enter a topic you want more information about.
Options button	Displays options you can use to change your view of Help
Menus	Contains commands to print help topics, close the Help window, and so on
Browse buttons (<< and >>)	Enables you to browse forward and back through help topics

Note Not all buttons are available in all help windows:

To keep the Help window on top of any other open windows:

1. In the Help window, click the Options button or menu.
2. Point to Keep Help On Top, and then click On Top.

Hypertext Links

You can move directly from one help topic to a related topic by clicking on a hypertext link. Any underlined text (green on a color monitor) in the Help window is a hypertext link.

Hypertext links can be:

- Words in a paragraph
- Topics listed at the end of a help topic

To jump to the topic indicated by the hypertext link, click the underlined text.

Using the Back Button

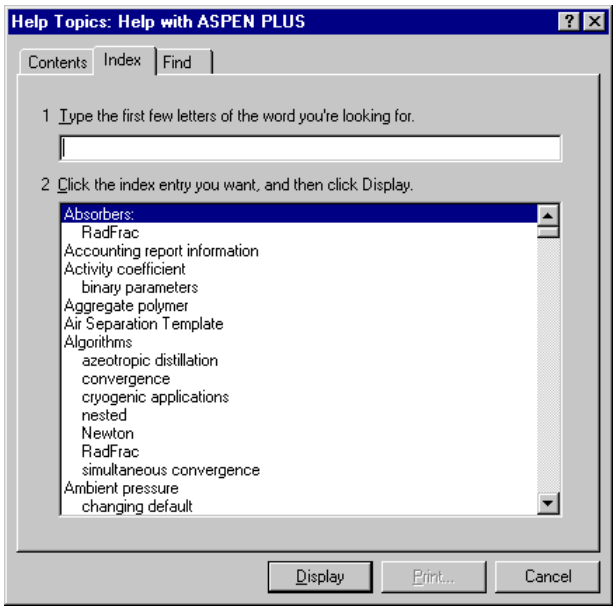
Use the Back button to move back through help screens you have seen. If there is no previous topic to view, the Back button is unavailable. Back keeps a complete record of all the help topics you view. This list is cleared each time you exit help.

Searching for Help on a Topic

You can find specific information quickly by searching for it. To search for a topic or keyword:

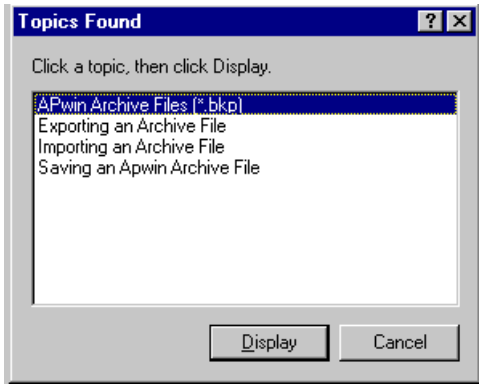
1. From the Help menu, click Help Topics, then click the Index tab.

   The Index dialog box appears:



2. Start typing a word or phrase to display a list of index entries that match what you are looking for.
3. Click Display or double-click on the entry in the list.

   Either the topic appears, or a dialog box containing a list of topics appears:



4. To display the topic you want, click the topic, then click Display.

   The help topic appears in the Help window.

Displaying Help on Dialog Boxes, Forms and Sheets

To access online Help that gives you an overview of a dialog box, form or sheet:

➤ Click the Help button on the dialog box, form or sheet.

– or –

Press F1 on the dialog box, form or sheet.

Displaying Help on Screen Elements

To access online Help on buttons, fields, commands on menus, and similar screen elements:

➤ Click the What's This button  or  on the window toolbar and then click the element.

– or –

Select the element, then press F1.

Getting Step by Step Help

To get help on preparing, specifying, and running simulations, and reviewing results:

1. From the Help Topics dialog box, click the Contents tab.
2. Double-click Using Aspen Plus, then click the topic you want.

Getting Reference Information

To obtain reference information:

➤ From the Help Topics dialog box, click the Contents tab, then click the appropriate topic.

Printing Help

To print a help topic:

1. Make sure the printer settings are correct.

   To check this, Click Start, then point to Settings then Printers.

2. Display the Help topic you want to print.
3. Click the Print button.

   – or –

   Click the Options button, then click Print Topic.

   – or –

   From the File menu, click Print Topic.

Printing Popup Help

To print popup help windows:

1. Click with the right mouse button on the Help window.
2. From the popup menu, click Print Topic.

Improving Help

We value your comments, suggestions, and criticisms. If you couldn't find the Help you were looking for, needed more assistance that the online help provided, or have any suggestions for future improvements to our online information, we want to know.

Please email your comments to **Docs@Aspentech.com**

Note If you have a query about Aspen Plus itself and want to email the AspenTech Support team, please email your local Technical Support office.

❖ ❖ ❖ ❖

4 Defining the Flowsheet

This chapter describes defining a process flowsheet in Aspen Plus including:

- Creating a process flowsheet
- Using heat and work streams
- Using pseudoproduct streams
- Viewing a process flowsheet
- Checking flowsheet completeness
- Modifying a process flowsheet
- Using flowsheet sections
- Printing

For descriptions and information about the user interface, see Chapter 1.

Creating a Process Flowsheet

To define a process flowsheet:

1. From the View menu, ensure that PFD mode is turned off. Otherwise, the blocks and streams you place graphically, do not become part of your simulation model. For more information, see Chapter 14.
2. Select the unit operation blocks and place them in the Process Flowsheet Window.
3. Connect the streams to the blocks.

After placing blocks and streams, you can:

- Delete blocks and streams
- Rename the blocks and streams
- Change stream connections

You can also improve the appearance of your flowsheet in many different ways. For more information, see Modifying the Flowsheet on page 4-11.

When you are defining your flowsheet, the shape of the mouse pointer changes, indicating the particular mode Aspen Plus is in:

Pointer Shape	Function	Use
	Select mode	Click an object to select it. Click and hold an object to enter Move mode. Click and drag to select a region or to move or resize a region (The pointer changes to the Resize shape).
	Insert mode	Click to place a model of the type selected in the Model Library. **Note** After placing each block, you remain in Insert Mode until you click the Select Mode button in the upper left corner of the Model Library.
	Connect mode	Click a port to connect the stream to it Click a blank area of the flowsheet to to place a feed or product
	Move mode	Click and hold to move the object to a desired location
	Port move mode	Click and hold to move the port to a desired location Drag the port away from the model to enter Disconnect mode
	Disconnect mode	Click and hold on a stream while dragging it away from a block to disconnect it. Release the mouse button to enter Connect mode.
	Resize mode	Click and drag to resize a model or region

Use the Model Library to select unit operation models to be used in the simulation.

Placing Blocks

To place a unit operation block in a simulation flowsheet:

1. Click a model category tab in the Model Library to display a list of models in that category.
2. In the Model Library, select the unit operation model that you want to place in your process flowsheet. To choose a different icon for the model, click the down arrow, and click an icon to select it. The icon you select will remain the default icon when placing that model, until you change the icon.
3. Click and hold down the mouse button on the unit operation model, and drag it to the Process Flowsheet window.
4. The mouse pointer is in the shape of a box with an arrow,  which indicates that only one block will be placed.

5. In the Process Flowsheet window, release the mouse button where you want to place the block.

   If you have switched off Automatically Assign Block Names, you are prompted to enter the Block ID. For more information on IDs, see Options for Naming Blocks and Streams on page 4-12. The icon that you selected appears on the flowsheet.

6. Continue creating your flowsheet. To place another block repeat steps 1 through 4.

   When you place or move blocks, the center of the block icon snaps to a grid location if Snap to Grid is enabled on the Grid/Scale tab of the Tools Options dialog box.

Placing Multiple Blocks

To place multiple blocks of the same type in the flowsheet:

1. Click a model category tab in the Model Library to display a list of models in that category.
2. In the Model Library, select the unit operation model that you want to place in your process flowsheet. To choose a different icon for the model, click the down arrow, and click an icon to select it. The icon you select will remain the default icon when placing that model, until you change the icon.
3. Click the unit operation model (click the icon then release the mouse button.)

   The pointer appears in the shape of a crosshair, representing Insert mode.

4. In the Process Flowsheet window, click where you want to place the block. The icon that you selected appears on the flowsheet.

   If you have switched off Automatically Assign Block Names, you are prompted to enter the Block ID. For more information on IDs, see Options for Naming Blocks and Streams on page 4-12. The icon that you selected appears on the flowsheet.

5. Continue creating your flowsheet.

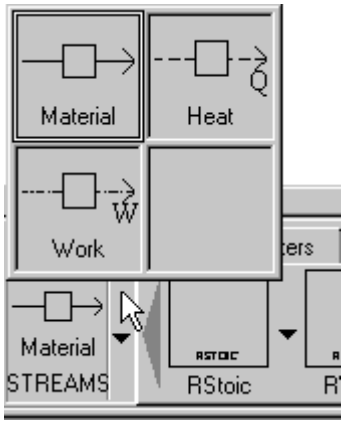
If you want to	Do this
Place another block for the same model	Click in a new location on the flowsheet.
Place a block for a different model	Repeat steps 1 to 4.
Stop placing blocks	Click the Select Mode button  in the upper left corner of the Model Library. This turns off insert mode. Insert mode is on when the Select Mode button is raised, and off when the button is depressed.

When you place or move blocks, the center of the block icon snaps to a grid location if Snap to Grid is enabled on the Grid/Scale tab of the Tools Options dialog box.

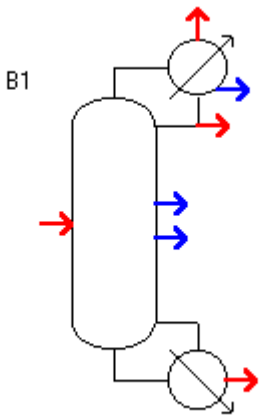
Placing Streams and Connecting Blocks

To place a stream:

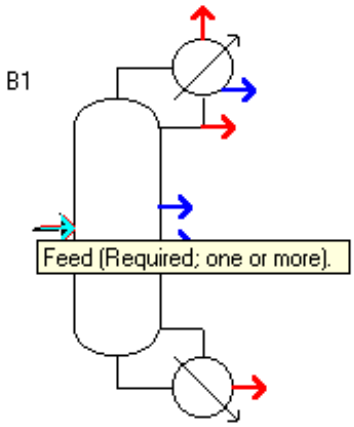
1. Click the STREAMS icon on the left side of the Model Library.
2. If you want to select a different stream type (Material, Heat or Work), click the down arrow next to the icon and choose a different type.



Move the mouse pointer to the Process Flowsheet window. For each block in the Process Flowsheet window, all ports that are compatible with that stream type are highlighted.



Ports that must have at least one stream connected are shown in red. Other optional ports are shown in blue. If you position the mouse over a displayed port, the arrow is highlighted and a text box with the description of the port appears.



3. Click a highlighted port to make the connection.

   If the port is not at the location you want it, click and hold the mouse button on the port. When the mouse pointer changes to the port move shape (↔↕) drag to relocate the port on the icon.

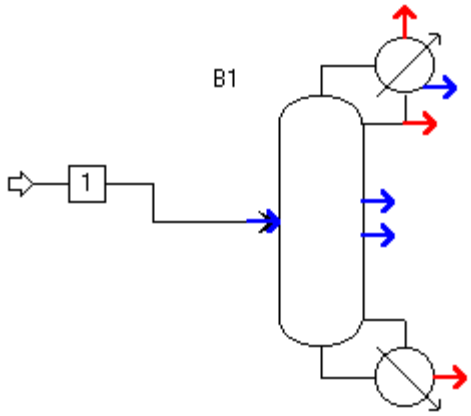
4. Repeat step 4 to connect the other end of the stream.

   Only those ports that you can connect the other end of the stream to remain highlighted. For example, if you connect a stream to an outlet port, inlet ports remain highlighted but outlet ports are no longer highlighted.

   If you have switched off Automatically Assign Stream Names on the Flowsheet tab of the Tools Options box, then you will be prompted for a Stream ID.

5. To place one end of the stream as either a process flowsheet feed or product, click a blank part of the Process Flowsheet window.

   If the stream's source is already connected, then a product will be placed. If the stream's destination is already connected, then a feed will be placed. By default, if you click a blank part of the window before connecting either stream end, a feed is placed.



6. To stop placing streams click the Select Mode button  in the upper left corner of the Model Library:

   To cancel connecting the stream at any time, press ESC or click the right mouse button.

   To place another stream of the same type, repeat steps 4 through 6.

   To place a stream of a different type, repeat steps 2 through 6.

You can also use drag and drop to connect streams. The procedure is similar to the one described above.

1. Select the stream type you want, by clicking the Material Stream icon in the Model Library or using the down arrow next to the icon to select a Heat or Work stream.
2. Click and hold down the mouse button on the stream icon.

   Tip Hold down the CTRL key during drag and drop to remain in Insert mode after completing connections for the first stream.
3. Move the cursor to the Process Flowsheet Window.

   The compatible ports are highlighted.
4. Release the mouse button on:
   - A port to make a connection
   - A blank part of the flowsheet to place a feed
5. Move the mouse and click:
   - Another highlighted port to connect the other end of the stream
   - A blank part of the flowsheet to place a product

Using Heat and Work Streams

You can define heat and work streams to transfer heat and power between blocks, or for duty and power specifications. For example, you can use a work stream to transfer power from a turbine to a compressor. For more information on Heat and Work streams, see Chapter 9.

When creating a heat or work stream:

- Select the heat or work icon from the Model Library.
- Use a port labeled Heat Stream(s) or Work Streams(s).

Heat and work streams appear as dashed lines in the flowsheet.

Using PseudoProduct Streams

You can define pseudoproduct streams to represent column internal flows, compositions, thermodynamic conditions streams for some unit operations models. For more information, see Chapter 9.

Pseudoproduct streams from one block may be an inlet to another block. Using a pseudo-stream as a block inlet results in an imbalance in the overall flowsheet material and energy balance report.

To define a pseudoproduct stream:

➤ When creating the stream select a port labeled Pseudo Streams.

Viewing The Flowsheet

If your flowsheet contains more than a few blocks, your workspace will soon be full.

Sometimes block and stream IDs appear off the screen, so it is difficult to locate a particular block or stream.

To display a block that is off the screen or a specific part of the flowsheet, you can use the:

- Zoom level
- Scrollbars
- Data Browser
- Bookmarks

- Pan

Adjusting the Zoom Level

To change your view of the flowsheet by zooming:

➤ From the View menu point to Zoom, then the option you require.

– or –

1. Position the mouse pointer in an empty area of the Process Flowsheet window and click the right mouse button.
2. From the menu that appears, click:

This zoom option	To
Zoom In	Zoom in
Zoom Out	Zoom out
Zoom Full	Show the full flowsheet

With the view zoomed in, you can display a specific part of the flowsheet by using the scroll bars.

Adjust the effect of Zoom In and Zoom Out by selecting Options from the Tools menu and changing the value of the Zoom Scale Factor on the Grid/Scale tab.

Using the Scrollbars

If you are working in a large flowsheet, the block you want to connect to may be off the screen. You can use the scrollbars to display:

- A block that is off the screen
- A specific part of the flowsheet

To use the Workspace scrollbars:

➤ Click a scrollbar arrow.

The amount that this moves the view is determined by the Scroll Step Size on the Grid/Scale tab of the Tools Options dialog box.

– or –

➤ Click between the slider and an arrow.

This moves the view by a set amount.

Using the Data Browser to Find Blocks in a Large Flowsheet

If you are working in a large flowsheet, it may be difficult to locate a particular block. You can use the Data Browser to find a block:

1. From the Data menu, click Data Browser (or press F8).
2. Expand the Blocks folder.
3. Select the block that you want to find.
4. Return to the Process Flowsheet window, without clicking it. To do this:

If you have/are in this view	Do this
Normal	From the Window menu, click Process Flowsheet window – or – Click the titlebar of the Process Flowsheet window
Flowsheet as Wallpaper	Minimize or close the Data Browser
Workbook	Click the Process Flowsheet tab

   The block you selected is highlighted.
5. Click the block with the right mouse button and from the menu that appears, click Center View.
6. Click an empty part of the flowsheet and click with the right mouse button, and from the menu that appears, click Zoom In if you want a closer view.

Using Bookmarks

If you are working in a large flowsheet, there may be sections that you want to look at frequently. Use Bookmarks to save these views.

To create a bookmark:

1. While in Select mode, click and drag to select an area of the flowsheet.
2. Click the right mouse button and from the menu that appears, click Bookmarks.
3. **Tip** You can also press F3 to access Bookmarks.
4. Type a name for the Bookmark in the Name box, then click Add to add the bookmark to this list.
5. To exit the Bookmarks dialog box, click Close.

To go to a bookmarked view:

1. In the Process Flowsheet window, click the right mouse button.

2. From the menu that appears, click Bookmarks.

   Tip You can also press F3 to access Bookmarks.

3. Click the name of the desired Bookmark, then click Go To.
4. The flowsheet appears in the predefined view you selected.

Using Pan

Use Pan to select a view of the flowsheet at the current zoom level.

1. In the Process Flowsheet window, click the right mouse button.
2. A full view of the flowsheet appears and a dashed rectangle.
3. Move the rectangle to an area that you wish to zoom in on and click the left mouse button.
4. To cancel pan, click the right mouse button.

Checking Flowsheet Completeness

To check completeness for the entire flowsheet, look at the status indicator in the bottom right of the main window.

If the status is *Flowsheet Not Complete*, then flowsheet connectivity is incomplete because:

- Additional streams must be connected to one or more blocks in the flowsheet.
- Streams have been disconnected but not reconnected.
- No blocks have been defined.
- To find out why the connectivity is incomplete:

➤ Click the Next button  on the Data Browser toolbar.

A Flowsheet Not Complete window indicates what is required to complete the flowsheet definition.

If any other status message appears, then flowsheet connectivity is complete. All required streams are connected to flowsheet blocks.

Modifying the Flowsheet

You can modify the flowsheet at any time to:

- Change its connectivity
- Improve the appearance
- Redraw all or part of the flowsheet

Changing Flowsheet Connectivity

To change the flowsheet connectivity, you can:

- Delete blocks and streams
- Rename blocks and streams
- Change stream connections
- Insert a block into a stream

Deleting Blocks and Streams

To delete a block or stream:

1. Click the block or stream to select it.
2. Click with the right mouse button on the block or stream.
3. From the popup menu that appears, click Delete Block or Delete Stream.
4. When prompted, click OK.

Tip You can also select the block or stream, then press Delete on the keyboard.

Renaming Blocks and Streams

To rename a block or stream from the flowsheet:

1. Select the block or stream you want to rename.
2. Click the right mouse button on the block or stream.
3. From the menu that appears, click Rename Block or Rename Stream.
4. When prompted, enter the new name and click OK.

You can also rename blocks and streams using the Data Browser.

Options for Naming Blocks and Streams

By default, Aspen Plus automatically assigns IDs to blocks and streams. You can either:

- Supply prefixes for the automatic naming
- Turn off the automatic naming and be prompted for a name for each block and stream as you place it

To specify the naming options:

1. From the Tools menu, click Options.
2. Click the Flowsheet tab.
3. Select the Automatically Assign Block Name with Prefix and/or Automatically Assign Stream Name with Prefix check box(es).
4. If desired, you can also type a prefix in the field. A sequential number is added to the prefix. If no prefix is supplied, the blocks or streams are numeric.

   For more information on flowsheeting options, see Chapter 16.

Changing Stream Connections

You can disconnect the end of a stream from a unit operation block and then connect it to another port on the same or a different block. To change the port that a stream is connected to:

Method 1:

1. Click to select the stream that you want to move or click the block to which the streams is connected.
2. Position the mouse pointer where the end of the stream connects to the block, so the arrow is highlighted and a text box with the name of the port appears.
3. Hold down the left mouse button and the mouse pointer changes to the port move shape.
4. Move the stream end away from the block. The mouse pointer changes to the disconnect shape indicating that the stream is about to be disconnected.
5. Click the mouse button to disconnect.

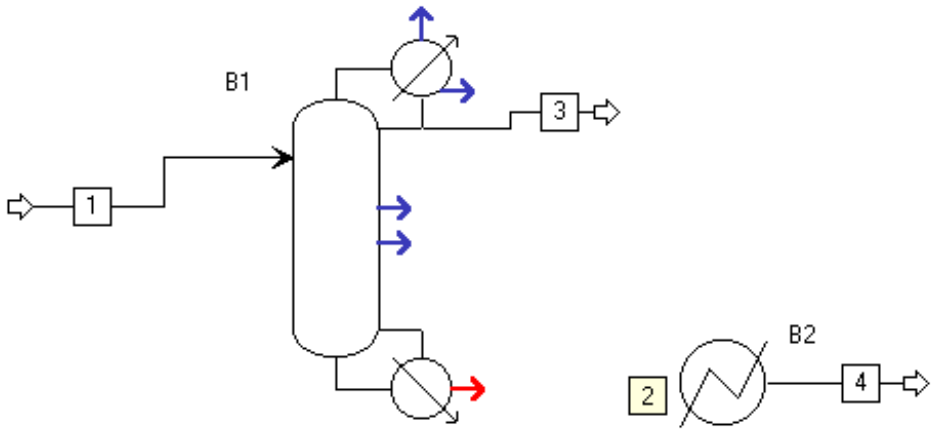
   For each block all available ports are highlighted. For example, for a feed stream, the outlet ports are highlighted. The ID of the stream appears in a text box by the end that is being reconnected. Ports that must have at least one stream connected are shown in red. Others are shown in blue.
6. Click the port to which you want to connect the stream end.

Method 2:

1. Click the stream.
2. Click the right mouse button.
3. From the menu that appears, click:

   - Reconnect Source to disconnect the source end of the stream
   - Reconnect Destination to disconnect the output end of the stream

   For each block all available ports are highlighted. For example, for a feed stream, the outlet ports are highlighted. The ID of the stream appears in a text box by the end that is being reconnected. Ports that must have at least one stream connected are shown in red. Others are shown in blue.



4. Continue as you would for a new stream. Click the port to which you want to connect the stream end, or click a blank part of the flowsheet to place a feed or product.

Inserting a Block into a Stream

To insert a block into a stream:

1. Place the new block on the flowsheet by selecting a unit operation model from the Model Library and dragging it to the flowsheet. For more information, see Placing Blocks on page 4-2.
2. Select the desired stream and click the right mouse button on the stream.
3. From the menu that appears, click Reconnect Source or Reconnect Destination.

4. Click a port on the new block to reconnect the stream to it.
5. Connect a new stream from the new block to the original source or destination, by clicking the STREAMS icon and clicking the inlet or outlet port. For more information, see Placing Blocks on page 4-2.

Improving the Appearance of the Flowsheet

You can change the flowsheet layout at any time to improve the appearance of your drawing. You can move:

- Blocks
- Multiple blocks and streams at once
- Block IDs
- Stream segments
- Stream corners
- Streams IDs
- Stream connnection locations

You can also:

- Hide block and stream IDs
- Reroute streams
- Align blocks
- Change icons
- Resize icons
- Rotate icons
- Use Place to redraw flowsheets automatically

Many commands and actions can apply to multiple blocks or streams as well as to an individual one.

You can select multiple blocks and streams in several ways:

- Click and hold the mouse button while dragging the mouse over a region.
- Hold down the Ctrl key while clicking on the blocks or streams.
- Click the right mouse button in the Process Flowsheet window. From the menu that appears, click Select All.

  Click here for information on moving multiple objects at once.

Moving Multiple Objects at Once

To move multiple objects at once:

1. Select the objects you want to move.
2. Hold down the mouse button on any object within the region.

The mouse pointer changes to the move shape (✥).

3. Drag the objects to the location you want, and release the mouse button.

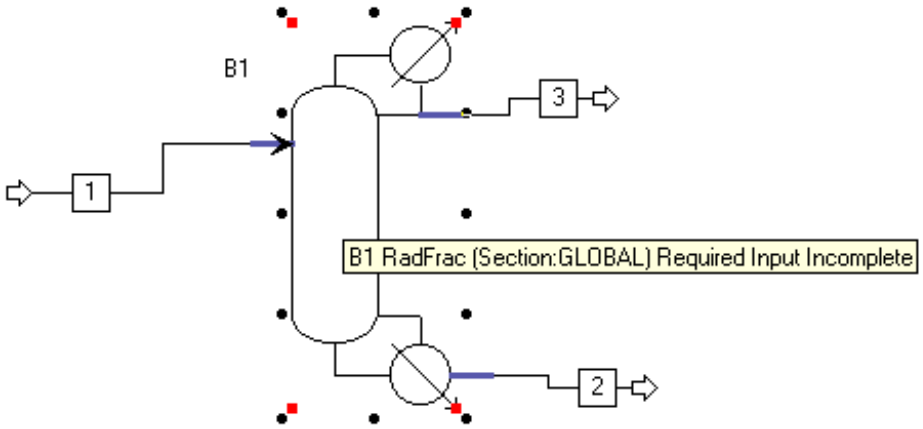
   Tip You can also select multiple objects and then use the arrow keys (←↑→↓) to move them to the new location.

Moving a Block

To move a block:

1. Press and hold down the mouse button on the unit operation block (but not on the block ID) that you want to move.

   The outline of the block is highlighted and the mouse pointer changes to the move shape. Also a text box appears showing information about the block, including name, section and status of the block.



2. Drag the block to the location you want and release the mouse button.

   When you place or move blocks, the center of the block icon snaps to a grid location if Snap to Grid is enabled. For information on changing the grid options, see Chapter 16.

   Tip You can also select the block and then use the arrow keys (←↑→↓) to make minor adjustments to the position of the block.

Moving a Block ID

To move a Block ID:

1. Press and hold down the mouse button on the block ID.

The mouse pointer changes to the move shape (✥).

2. Drag the block to the location you want and release the mouse button.

   Tip You can also select the block ID and then use the arrow keys (←↑→↓) to move the block ID.

   If you later move the block, the ID maintains its position relative to the block.

Hiding a Block or Stream ID

To hide a block or stream ID:

1. Click the block or stream in the flowsheet to select it.
2. From the Flowsheet menu, point to Hide and then ensure ID is checked.

   – or –

   Click the right mouse button and from the menu that appears, point to Hide and then ID.

   – or –

   Press CTRL + H on the keyboard.

   Tip To hide the block IDs for all future blocks created, clear the Display Block Name checkbox on the Flowsheet tab of the Tools Options dialog box. For more information, see Chapter 16.

Changing the Icon

To change an icon:

1. Click the block whose icon you wish to change.
2. Click with the right mouse button on the block.
3. From the popup menu that appears, click Exchange Icon.
4. The icons for the block changes to the next icon in the list for the model.

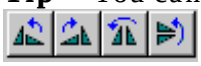
   Tip You can also change the icon by clicking the block, then pressing the letter n to change to the next icon available for the block, or p to change to the previous available icon.

Rotating Icons

To rotate an icon:

1. Click the block whose icon you wish to rotate.

2. Click with the right mouse button on the block.
3. From the menu that appears, click Rotate Icon.
4. A submenu appears, allowing you to rotate the icon to the right (clockwise) or left, or flip the icon around either axis (for example, to reverse flow direction).

   Tip You can also use the buttons on the Process Flowsheet toolbar  to rotate and flip an icon.

Resizing Icons

To resize an icon:

1. Click the block whose icon you wish to resize.
2. Click with the right mouse button on the block.
3. From the menu that appears, point to Resize Icon, then Shrink or Enlarge to shrink or enlarge the icon by a built-in factor.

   – or –

   Position the mouse pointer over one of the corners of the block icon until the Resize mode pointers appear. Drag the mouse pointer until the icon until it is the desired size.

Aligning Blocks

To align two blocks:

1. Click the stream between the two blocks.
2. Click with the right mouse button on the stream.
3. From the menu that appears, click Align Blocks.

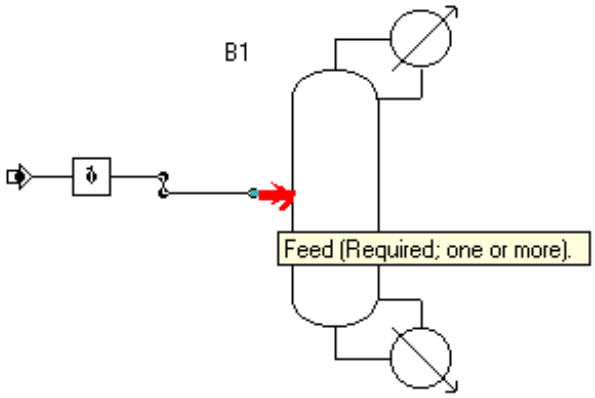
   Tip You can also select one or more streams and press CTRL + B.

Note Blocks attached to selected streams are aligned on a grid if Snap to Grid is enabled on the Grid/Scale tab. For information on this, see Chapter 16.

Moving Stream Connection Locations

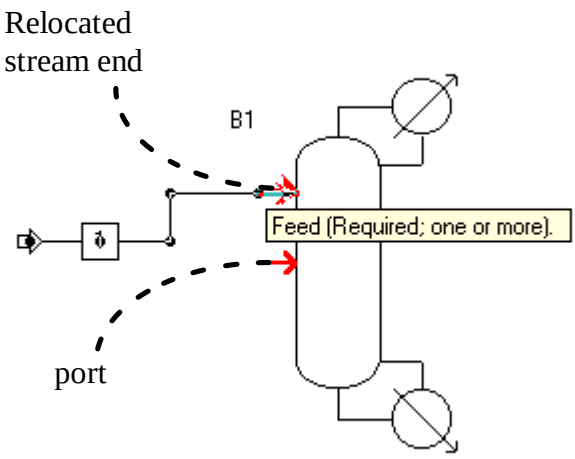
To move the point where a stream connects to a unit operation block without changing the stream's connection to its current port on the icon:

1. Click the stream that you want to move or click the block to which it is connected. The stream is selected.



2. Position the mouse pointer where the end of the stream connects to the block.
3. The arrow is highlighted and a text box with the descriptions of the port appears.
4. Hold down the left mouse button. The mouse pointer changes to the move shape.
5. Drag the stream end to the preferred point on the block and release the mouse button.

   Moving the stream end does not move the port to which the stream is connected. Consequently, the point where the stream end is now attached to the block is not a port and may not be used to directly connect further streams.
6. To display the location of the port, click the stream end:



Tip You can also move any part of the stream by selecting it and dragging the part of the stream you want to move to its new location.

Moving a Stream Segment

To move a stream segment:

1. Press and hold down the mouse button on the segment of the stream you wish to move (but not on the stream ID).
2. The mouse pointer changes to the move shape.
3. Drag the segment of the stream to the location you want and release the mouse button.

   Tip You can also select the stream and then use the arrow keys (←↑→↓) to make minor adjustments to the position of the stream.

Moving a Stream Corner

To move a stream corner:

1. Press and hold down the mouse button on the corner of the stream (but not on the stream ID).

   The mouse pointer changes to the move shape.
2. Drag the corner of the stream to the location you want and release the mouse button.

   Tip You can also select the stream and then use the arrow keys (←↑→↓) to make minor adjustments to the position of the stream.

Moving a Stream ID

You cannot move a stream ID off a stream but you can move a stream ID along a stream. To do this:

1. Press and hold down the mouse button on the stream ID, until the mouse pointer changes to the move shape ().
2. Drag the block to the location you want and release the mouse button.

Rerouting Streams

To reroute a stream automatically:

1. Click the stream you wish to reroute.
2. Click the right mouse button on the stream.
3. From the menu that appears, click Reroute Stream.

Tip You can also select one or more streams and then press CTRL + J to reroute them.

Using Place and Unplace to Redraw the Flowsheet

When you want to make several changes to the layout of all or part of a flowsheet, you might find it easier to temporarily remove (unplace) one or more blocks and then replace them.

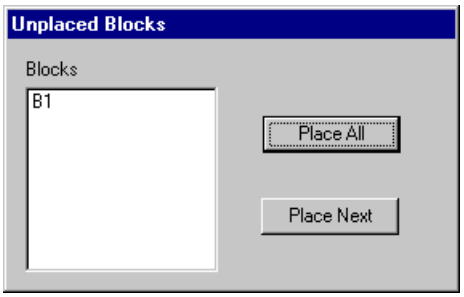
To do this, use Place and Unplace to redraw all or part of the flowsheet at any time. You can place:

- All of the blocks at once and let Aspen Plus choose the layout
- Blocks one at a time to create the layout you want

Before you can redraw the flowsheet, you need to temporarily remove (or unplace) one or more blocks:

To remove	Do this
A group of blocks	Select a group of blocks. Click the right mouse button on one of the blocks and from the menu that appears, click Unplace Blocks.
A single block	Select a block. Click the right mouse button and from the menu that appears, click Unplace Blocks.

The unplaced blocks appear in the Unplaced Blocks dialog box.



Tip You can also select one or more blocks and then press CTRL + U to unplace them.

Using Place to Place a Block on the Flowsheet

Use Place to place an individual block on the flowsheet. Do this when you want to achieve a specific layout.

To place an unplaced block on the flowsheet yourself:

1. In the Unplaced Blocks dialog box, click and hold down the mouse button on the ID of the block that you want to place.

2. Drag the block to the flowsheet and drop it where you want the block located.

If you want Aspen Plus to place the next block automatically:

➤ In the Unplaced Blocks dialog box, click Place Next.

Aspen Plus selects the block that logically should appear next in the flowsheet and places it in the appropriate position. This will not necessarily be the block listed first in the Unplaced Blocks dialog box.

If you do not like where Aspen Plus has placed the block, move it to a different location.

As you place blocks, the streams that connect them also appear. You can move stream segments or corners to achieve the desired routing.

Using Place All to Place All the Blocks at Once

If the number of unplaced blocks is small or you are not concerned about the layout of the flowsheet, you can place any unplaced blocks quickly by using Place All to place all the blocks on your flowsheet at once.

Aspen Plus chooses the layout for you.

To place all the blocks at once:

1. Select a block or group of blocks.
2. Click the right mouse button.
3. From the popup menu that appears, click Unplace Blocks.
4. In the Unplaced Blocks dialog box, click Place All.
5. Move individual blocks and reroute streams if necessary.

About Flowsheet Sections

A flowsheet section is a group of blocks and streams within the flowsheet. Use flowsheet sections to:

- Enhance clarity
- Simplify viewing and printing large flowsheets
- Simplify assignments of physical property specifications or stream classes

A stream belongs to a flowsheet section if it is an outlet of a block in the section. A process feed stream belongs to a section if it is an inlet to a block in the section.

To see which section a block or stream belongs to, select the block or stream and a text box with the information will be displayed while the pointer is over the selected item.

Aspen Plus predefines a default section GLOBAL for your convenience. It assigns all blocks to GLOBAL unless you create additional sections.

Use the Properties Specifications Flowsheet Section sheet to specify physical property options for sections.

The remaining sections of this chapter describe how to create and use flowsheet sections.

Creating a Flowsheet Section

To create a new flowsheet section:

1. From the Flowsheet menu, click Flowsheet Sections.
2. On the Flowsheet Sections dialog box, click New.
3. Enter an ID or accept the default ID then click OK.

The new section becomes the current section. Any additional blocks you create are assigned to this section, until you select a new current section.

Tip You can use this button  on the Section toolbar to quickly open the Flowsheet Sections dialog box.

Specifying the Current Section

The current section is shown by the Section box on the Section toolbar. All new blocks defined using graphics are assigned to the current section.

To change the current section:

1. From the Flowsheet menu, click Flowsheet Section.
2. In the Flowsheet Sections dialog box, select a section from the list or click the New button and create a new section.
3. Click the Make Current button.
4. Click OK to close the Flowsheet Sections dialog box.

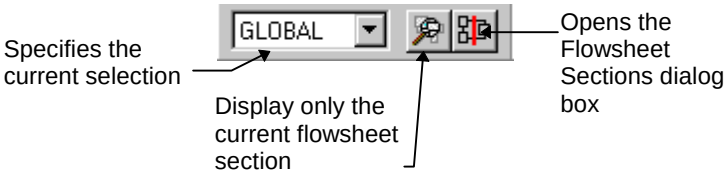
The section you selected becomes the current section. Any additional blocks you create are assigned to this section, until you select a new current section.

Tip You can use the current section list 

on the Section toolbar quickly specify the current section.

Using the Section Toolbar

The Section toolbar can be used to quickly change some options on the flowsheet sections.



Moving Blocks to a New Section

To move blocks from one section to another:

1. In the Process Flowsheet window, select one or more blocks.
2. Click the right mouse button on a selected block and from the menu that appears, click Change Section.
3. To move the block or blocks to a different section, select the Move to section option and select a section from the list.

   – or –

   To create a new section, select the Create new section option and enter a section ID or accept the default ID.
4. Click OK to close the Change Section dialog box.

   The selected block or blocks are moved to the section you selected or created.

Specifying the Stream Class for a Section

The stream class assigned to section GLOBAL is the default stream class. By default, Aspen Plus assigns the stream class for section GLOBAL to any new sections you create.

To assign a different stream class to a section:

1. If the stream class you want to assign to the section does not contain the appropriate substreams, use the Setup StreamClass form to modify it. For more information, see Chapter 5.
2. From the Flowsheet menu, click Flowsheet Sections.
3. In the Flowsheet Sections dialog box, do one of the following:
   - Select a section from the list
   - Click the New button and create a new section
4. Click the Stream class button.
5. Select a stream class using the list. Click OK.

You can also use the Setup Specifications Global sheet to assign the GLOBAL stream class.

Viewing the Current Section

To view only the current section:

1. Click the Process Flowsheet window.
2. From the View menu, click Current Section Only.

Only the blocks and streams in the current section appear on the screen. Streams to and from other sections are terminated by icons containing the ID of the other sections.

To specify what is the current section see Specifying the Current Section on page 422.

Tip You can use the  button on the Section toolbar to quickly view only the current Flowsheet Section.

Printing a Flowsheet

To print a flowsheet:

1. Click in the Process Flowsheet Window to make it active.
2. Click the Printer button on the Standard toolbar.

   – or –

   From the File menu, select Print.
3. Choose the printer and desired settings in the Print dialog box.

4. Click OK.

Printing a Section of Flowsheet

To print a section of flowsheet:

1. From the Flowsheet menu, click Flowsheet Sections.
2. Choose the flowsheet section you want to print and click OK.
3. From the View menu, click Current Section Only.
4. Click the Printer button on the toolbar.

   – or –

   From the File menu, select Print.
5. Choose the printer and desired settings in the Print dialog box.
6. Click OK.

For more information on printing, see Chapter 14.

❖ ❖ ❖ ❖

5 Global Information for Calculations

This chapter explains how to specify and change all types of global information, including:

- About global information
- Entering global specifications
- Overriding default simulation options
- Units of measure
- Report options

About Global Information

Global specifications establish defaults for an entire run. Specify global information before entering any engineering specifications for your Aspen Plus run.

You can override these defaults for specific objects on other sheets. Although you can return to these forms and change entries at any time, it is recommended that you use them before any others when starting a new run.

Enter global specifications on the Setup forms. To access the Setup forms:

1. From the Data menu, click Setup.
2. The following table shows which form to use to enter information:

Use this form	To
Specifications	Enter global information
Simulation Options	Specify calculations, flash convergence, and system options, and time and errors limits
Stream Class	Define stream class and stream properties
Substream	Define substreams and attributes
Units Sets	Define units-of-measurement sets
Report Options	Specify report options

All of the global information you normally need to specify is on the Setup Specifications Global sheet. When you create a new run, the Application Type you choose establishes the defaults for the Global sheet. The Aspen Plus expert system takes you to the Global sheet so you can view the defaults and change or supplement them if you want to. For most simulations, it should not be necessary to change the defaults on the other Setup sheets.

Entering Global Specifications

Use the Setup Specifications form to enter global specifications, accounting report information, diagnostic levels, and a run description for reports. The following table shows the information you can enter on each sheet:

On this sheet of the Specifications form	Enter this information
Global	Run type, run title, run description, global defaults (units, flow basis, phase equilibrium, calculation options, stream class)
Accounting	Run accounting information (required at some installations)
Diagnostics	Simulation history and Control Panel diagnostic message levels
Description	User supplied description of the simulation problem

Global Sheet

Use this sheet to enter a run title, specify default input and output units of measurement for the run, and specify global settings. The global settings include Run Type, Input Mode, Stream Class, Flow Basis, Ambient Pressure, Valid Phases, and Use Free Water Calculation.

You can override global specifications for individual unit operations blocks using the Block Options form for each block.

Changing the Run Type

You specify a Run Type when you create a new run. You can change this run type at any time.See Chapter 2 for a description of the available run types.

To change the run type:

1. On the Data menu, select Setup.
2. Click the Global sheet.
3. In the Run-Type box, select a run type.

Because each run type has different input requirements, changing the run type may cause the input for the run to become incomplete. Use Next to guide you through the required forms.

You can change the run type even after you have entered specifications for a different run type. Aspen Plus hides forms that the new run type does not allow. But if you switch back to the original run type, data entered on these hidden forms are not lost.

Examples of when you might want to change the run type are:

- You used a Property Estimation run to estimate and examine properties for a non-databank component. Now you want to run a flowsheet simulation using that component. If you change the run type to Flowsheet, Aspen Plus retains the component information and prompts you for the flowsheet information.
- You used a Property Estimation run to estimate and examine properties for a non-databank component. Now you want to run property analysis or property data regression involving that component. If you change the run type to Property Analysis or Data Regression, Aspen Plus retains the component information, and prompts you for additional information to complete your run specifications.

Specifying the Run Title

To specify the run title:

1. From the Data menu, click Setup.
2. Select the Global sheet.
3. In the Title box, specify a brief run title.

You can supply additional descriptive information about the run on the Setup Specification Description sheet, and on the Comment forms available from any input sheet.

Specifying Global Units Sets

You can specify separate global input and output units sets. For more information about how to customize an existing unit set, see Units of Measure on page 5-16.

This global units set	Becomes the default for all
Input Data	Input sheets in the run
Output Results	Results sheets

To specify global units sets:

1. From the Data menu, click Setup.
2. Select the Global sheet.
3. Specify the global units sets in the Input data and Output results boxes.

You can change the global units set specifications at any time. When you change the Input Data set, all new input forms you display default to the new units set. Aspen Plus does not change the units on forms you have already completed. When you change the Output Results units set, all results sheets default to the new units set after you complete a run.

Selecting a Default Stream Class

Stream classes define structures for simulation streams when solid substreams are present. When you create a new run, Aspen Plus chooses a default stream class based on the application type. You can change the default stream class on the Setup Specifications Global sheet.

To change the default stream class:

1. From the Data menu, click Setup.
2. Select the Global sheet.
3. In the Stream Class box, select a stream class.

All streams in the simulation are assigned to the default stream class, unless you assign a stream class to one of the following:

- A flowsheet section
- An individual stream, on the Stream-Class Streams sheet

For more information on using and creating stream classes, see Chapter 9.

Selecting the Simulation Flow Basis

You can enter specifications for most flows on a molar, mass, or standard liquid volume basis. For example, you can enter total stream flow rate on any of these bases.

To select the global basis for flow-related information:

1. On the Data menu, select Setup.
2. Select the Global sheet.
3. In the Flow-Basis box, specify Mass, Mole, or StdVol.

The basis you select becomes the default basis for the run. You can override the basis locally on most forms.

You can return to the Setup Specifications Global sheet and change the default basis at any time. The basis for previously entered values does not change.

Specifying Ambient Pressure for Gauge Pressure Units

Aspen Plus accepts gauge pressure units for all pressure variables. The default value for the ambient pressure is 1 atm.

To change the ambient pressure:

1. From the Data menu, click Setup.
2. Select the Global sheet.

3. In the Ambient Pressure box, type a pressure. Change the units if necessary.

Specifying Valid Phases

Aspen Plus performs phase equilibrium calculations throughout a simulation run for blocks, streams, and other objects. You can specify the valid phases to be used in these calculations. Choose from Vapor-Only, Liquid-Only, Vapor-Liquid, and Vapor-Liquid-Liquid.

To change the valid phases:

1. From the Data menu, click Setup.
2. Select the Global sheet.
3. In the Valid phases box, select either Vapor-Only, Liquid-Only, Vapor-Liquid, or Vapor-Liquid-Liquid.

You can override the global setting locally, at the individual block or stream level, using the Valid Phases box.

Requesting Free Water Calculations

Aspen Plus can handle the presence and decanting of water as a second liquid phase in water-hydrocarbon systems. Free-water calculations:

- Assume the water phase is pure
- Use special methods for calculating the solubility of water in the organic phase

To request free-water calculations globally:

1. From the Data menu, click Setup.
2. Select the Global sheet.
3. Select the Use Free Water Calculations check box.

You can override the global setting locally, at the individual block or stream level, using the Valid Phases box to select Vapor-Liquid-Free Water.

Description Sheet

Use this sheet to enter the description for the simulation. The description you enter on this sheet will be printed once, at the beginning of the report. You can enter any amount of text in uppercase and lowercase letters to document your run in more detail. You can use any number of lines to enter text. However, you cannot exceed the maximum length of each line (72 characters): the excess will be truncated.

Specifying a Run Description

To specify a run description:

1. From the Data menu, click Setup.
2. Select the Description sheet on the Setup Specifications form.
3. Enter a description in the Description box.

Tip You can write a description in your text editor (for example, Notepad), and then copy and paste them onto the Description sheet.

Accounting Sheet

Use this sheet to enter run accounting information (required at some installations). The accounting information includes: a user name, an account number, a project ID, and a project name. This information is stored for the run by the Aspen Plus Run Accounting System, if it is active for your installation.

Accounting Report Information

Accounting report information tracks the use of Aspen Plus at your installation. This information may be required at some installations.

To specify run accounting information:

1. From the Data menu, click Setup.
2. Select the Accounting sheet on the Setup Specifications form.
3. In the User Name box, specify a username.
4. In the Account Number box, specify an account number.
5. In the Project ID box, specify a project ID.
6. In the Project Name box, specify a project name.

The Aspen Plus Run Accounting System logs this information for the run, if it is active for your installation.

Diagnostic Sheet

Aspen Plus writes progress and diagnostic messages to the Control Panel and the History File during a run. The default for all types of messages is level 4. You can control the amount of diagnostic information produced, although it is generally not necessary. It is sometimes necessary to increase the level in order to converge a flowsheet or to debug user Fortran.

Use this sheet to override defaults for simulation history diagnostic message levels and Control Panel message levels printed. You can set message levels and diagnostics for input translation, simulation, physical properties, stream, convergence, Fortran variables, cost and economics.

Specifying Global Defaults for Diagnostic Information

To specify global defaults for diagnostic information:

1. From the Data menu, click Setup.
2. Click the Diagnostics sheet.
3. Use the slider controls to adjust the message levels you want to change. The slider on the top of each line is for the Control Panel messages, and the slider on the bottom is for the History File messages.
4. Click the History Options button to change the print options for the History file. Check Insert files used in the simulation or Sorted input if this information is desired in the History file.

Tip You can override the global defaults locally, using the Block Options sheets for streams, blocks, property tables, and other objects that perform calculations.

Setup Simulation Options

Use the Setup Simulation Options form to override defaults for simulation options set by Aspen Plus. Aspen Plus provides defaults for performing energy balances and convergence calculations. Aspen Plus also has default time limits. You can use this form to override these defaults. You also can specify simulation options at the individual block level.

This table shows which sheets are used for which information:

Sheet	Information
Calculations	Options for Heat and mass balances, molecular weight from formula, reinitialize calculations, bypass Prop-Set calculations, reaction stoichiometry checking
Flash Convergence	Global temperature and pressure limits, maximum iterations, flash tolerance, extrapolation threshold for equations of state
System	Interpret or compile Fortran, unit operation model and Fortran error checking
Limits	Simulation time and error limits

Calculations Sheet

Use this sheet to specify calculation options for:

- Checking mass balances around blocks
- Performing mass-balance-only calculations
- Calculating component molecular weight from atomic formula
- Using results from a previous convergence pass
- Bypassing prop-set calculations if flash fails

You can also use this sheet to specify reactions stoichiometry error checking options.

Checking Mass Balances Around Blocks

Aspen Plus performs a mass balance check around each block as it is executed and at the end of the simulation. Mass balance checking is performed with a relative tolerance of 0.0001.

Imbalances can occur for numerous reasons — for instance, improper stoichiometry or yield fraction specifications, loose convergence tolerances, inconsistent user kinetic rates, or flows changed by Fortran, Transfer, or Balance blocks. Mass balance checking will point out these imbalances and in many cases provide the reason for the imbalance.

You can turn off this checking to lower the number of error or warning messages generated during a simulation. To disable mass balance checking around blocks:

1. From the Data menu, click Setup.
2. In the left pane of the Data Browser window, select the Simulation Options form.
3. Click to clear the Check Mass Balance Error Around Blocks check box.

About Mass-Balance-Only Simulations

Mass-balance-only simulations:

- Are appropriate when energy balances are not required
- Do not calculate enthalpies, entropies, or free energies, thus reducing calculation time
- Reduce data input requirements for physical property parameters

Mass-balance-only simulations do not require:

- CPIG, DHFORM, and DGFORM parameters
- Parameters for models that calculate only enthalpy, entropy, or free energy

To request a mass-balance-only simulation:

1. From the Data menu, click Setup.
2. In the left pane of the Data Browser window, select the Simulation Options form.
3. Click to clear the Perform Heat Balance Calculations check box.

In a mass-balance-only run, you can use these unit operation models without restriction:

CFuge	HyCyc
Crusher	Mixer
Cyclone	Mult
Dupl	Screen
ESP	Sep
FabFl	Sep2
Filter	SSplit
FSplit	VScrub

You can use these models only if you do not specify heat duty:

CCD	RBatch
Decanter	RCSTR
Distl	RPlug
DSTWU	RSstoic
Flash2	RYield
Flash3	SWash
Heater	

You cannot use these models in a mass-balance-only run:

BatchFrac	PetroFrac
Compr	Pipeline
Crystallizer	Pump
Extract	RadFrac
HeatX	RateFrac
MCompr	REquil
MHeatX	RGibbs
MultiFrac	SCFrac

Heat and work streams are not allowed in a mass-balance-only simulation.

Calculating Molecular Weight from Formula

The molecular weight is available in Aspen Plus databanks (parameter MW). However, the databank molecular weight value may not contain enough significant figures for certain applications for which atomic balance is important, such as reactor modeling.

Aspen Plus calculates the molecular weight for all components in the simulation from the molecular formula (parameters ATOMNO and NOATOM) and the atomic weight. The calculated molecular weight is more accurate than the databank molecular weight. By default, the calculated molecular weight is used in the simulation.

To request to calculate from the formula in a simulation:

1. From the Data menu, click Setup.
2. In the left pane of the Data Browser window, select the Simulation Options form.
3. Click the Calculate Component Molecular Weight from Atomic Formula check box.

Reinitializing Calculations

By default, iterative calculations in Aspen Plus use any available previous results as an initial guess. If necessary, you can override this default and request that all calculations be reinitialized each calculation pass.

Request reinitialization when:

- A block has multiple solutions and you can obtain the one you want only by starting from your own initial estimate.
- A block or flowsheet fails to converge for no apparent reason, after one or more successful passes.

To request reinitialization globally:

1. From the Data menu, click Setup.

If the Use Results from Previous Convergence Pass check box is	Then Aspen Plus
Selected	Uses results from a previous calculation pass as the initial guess for the new pass
Clear	Performs initialization or uses initial estimates at every new calculation pass

You can override the global setting:

- At the block level, on the Block Options sheet for the block
- Interactively, using the Reinitialize commands from the Run menu
- If the reinitialization option for a block is clear when you request reinitialization interactively, reinitialization occurs only on the next calculation pass.

Bypassing Prop-Set Calculations When Flash Fails

1. By default, Aspen Plus will not calculate the property sets if a flash error occurs. In the left pane of the Data Browser window, select the Simulation Options form.
2. On the Calculations sheet, click to clear the Use Results from Previous Convergence Pass check box.

If the property sets are calculated when severe flash errors occurs, the property set calculations may be unreliable, and may cause further errors.

To request to calculate the prop-set calculations even when the flash fails:

1. From the Data menu, click Setup.
2. In the left pane of the Data Browser window, select the Simulation Options form.
3. On the Calculations sheet, clear the Bypass Prop-Set Calculations if Flash Failure Occurs checkbox.

Checking Reaction Stoichiometry

If reactions stoichiometry (such as Reactors, Chemistry, Reaction) is specified, Aspen Plus checks the mass-balance of stoichiometry based on the stoichiometric coefficient and molecular weight of the components.

You can use the option button to select whether Aspen Plus gives an error or a warning during Input translation if mass imbalance occurs. Simulation will not proceed if an error occurs during Input translation.

You can also use the Mass Balance Error Tolerance box to specify the absolute tolerance of the mass balance check of stoichiometry. The default value of the tolerance is 1 kg/kgmole.

The error severity depends on the Mass Balance Error Tolerance and what checking option you specify:

Checking Option	Absolute Error	Error Severity
Issue Error When Mass Imbalance Occurs	> Tolerance	Error
Issue Error When Mass Imbalance Occurs	< Tolerance and > 0.01	Warning
Issue Warning When Mass Imbalance Occurs	> Tolerance	Warning

To request a warning rather than an error to be issued when a mass imbalance occurs:

1. On the Data menu, click Setup.
2. In the left pane of the Data Browser window, click the Simulation Options form.
3. On the Calculations sheet, select the Issue Warning when Mass Imbalance Occurs check box.
4. The tolerance can be changed by typing a new tolerance in the Mass Balance Error Tolerance box.

Flash Convergence Sheet

Use the Flash Convergence sheet to specify calculation options for setting:

- Upper and lower limits of temperature for flash calculations
- Upper and lower limits of pressure for flash calculations
- Flash options for flash calculations
- Extrapolation threshold for equations of state

Specifying Temperature and Pressure Limits

To specify upper and lower limits on the temperature and pressure variables used in iterative flash and distillation calculations:

1. From the Data menu, click Setup.

2. In the left pane of the Data Browser window, select the Simulation Options form.
3. Select the Flash Convergence sheet on the Simulation Options form.
4. Use the Lower Limit and Upper Limit boxes to specify upper and lower limits for temperature and pressure.

These limits apply to the entire simulation. You cannot override them locally.

Specifying Global Flash Options

Aspen Plus performs phase equilibrium (flash) calculations throughout a simulation run, for blocks, streams, and other objects. You can specify global values for the maximum number of iterations and the convergence tolerance to be used in these calculations.

The flash tolerance may need to be tightened (lowered) in complex simulations with a number of recycle loops in order to help the convergence. For more information on convergence, see Chapter 18.

To specify global flash options:

1. From the Data menu, click Setup.
2. In the left pane of the Data Browser window, select the Simulation Options form.
3. Select the Flash Convergence sheet.
4. In the Maximum Number of Iterations box, specify the default for the maximum number of flash iterations.
5. In the Tolerance box, specify the default flash tolerance.

You can override the maximum number of flash iterations and flash tolerance on forms for blocks, streams, and other calculations.

Specifying Extrapolation Threshold for Equations of State

All equations of state in Aspen Plus use a root finder to calculate the molar volume iteratively at given temperature, pressure and mole fractions. Given physically meaningful conditions, the real molar volume root can always be located by the root finder. However, during iterative calculations in flash or a distillation model, the temperature, pressure, compositions and phase specification may be such that a real molar volume root does not exist. Aspen Plus provides an estimate of the molar volume that is reasonable, allowing the flash or distillation algorithm to converge to a physically meaningful solution.

If you encounter convergence problems due to extrapolation of an equation of state root finder, you can improve performance by changing the extrapolation threshold. A smaller value of the threshold makes it less likely for the extrapolation to occur.

To specify the extrapolation threshold for equations of state:

1. From the Data menu, click Setup.
2. In the left pane of the Data Browser window, select the Simulation Options form.
3. Select the Flash Convergence sheet.
4. In the Extrapolation Threshold for Equation of State box, specify a value for the extrapolation threshold.

This limit applies to the entire simulation. You cannot override it locally.

System Sheet

Use this sheet to override the defaults for system options that affect error checking and handling of in-line Fortran statements:

You can override these defaults:

- Interpret all in-line Fortran statements at execution time
- Compile all Fortran statements into the Aspen Plus main program
- Check unit operation block for errors and inconsistencies
- Print Fortran tracebacks when a Fortran error occurs

Limits Sheet

Use this sheet to specify limits for:

- Maximum CPU time for a batch run
- Maximum number of severe errors for a batch run
- Maximum number of Fortran errors for a batch run
- Maximum number of errors and warnings printed in the History file

Units of Measure

Use the Units Sets form to create new user-defined units sets and to view existing units sets. A units set is a collection of units for each dimensional quantity in Aspen Plus.

A units set defined using this form can be specified in the Input Data or Output Results boxes on the Setup Specifications Global Sheet or on the Units box on the toolbar of the Data Browser.

Sheet	Information
Standard	List and select an existing units set as a base for a new units set; search for all the dimensional quantities alphabetically; specify flow, temperature, and pressure-related units
Heat	Specify enthalpy, heat, heat capacity, and entropy-related units
Transport	Specify volume, density, transport-related and miscellaneous thermo units
Concentration	Specify energy/power, time, concentration, and composition-related units
Size	Specify size, equipment sizing, cost, and column sizing-related units
Miscellaneous	Specify miscellaneous units

Selecting Units of Measure

A units set is a collection of units specifications for each dimensional quantity used in Aspen Plus. Aspen Plus provides these basic units sets:

- International system units (SI)
- English engineering units (ENG)
- Metric engineering units (MET)

Additional built-in units sets are available, depending on which Application Type you choose when you create a new run.

In Aspen Plus you have complete flexibility in specifying units of measure. You can specify units on three different levels:

Level	For	For input sheets	For results sheet
Global units sets	Entire run	Yes	Yes
Sheet units set	Individual form or object	Yes	Yes
Field units	Individual fields or a group of fields	Yes	Yes

Viewing Units Specifications

To see what units are specified by a units set:

1. From the Data menu, click Setup.
2. In the left pane of the Data Browser window, select the Units Sets folder.
3. In the Units Sets object manager, select the units set you want to view and click Edit.

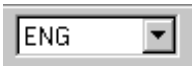
   The unit types used by Aspen Plus appear on six sheets: Standard, Heat, Transport, Concentration, Size, and Miscellaneous.
4. Select a sheet and view the units specifications.

You can create your own units sets on the Setup Units Set sheets. The following sections describe how to specify units for each level, andhow to define your own units set.

Specifying Units Sets for Forms or Objects

You can override the global units sets for individual forms and objects, such as for a block, stream, or property table. To do this:

➤ On the Data Browser toolbar, use the Units box to select a units set.



A units set specification applies to all forms for an object.

For example, if you specify a units set on the Data Browser toolbar while the RadFrac Setup Streams sheet is active, the new units set applies to all input forms for the block. For each object, you specify units sets separately for input forms and results forms.

Specifying Units Sets for Fields

You can specify units for individual fields and groups of fields on an input form. Selects units in the units fields next to the data fields.

Changing the units for an individual data field does not convert any value entered previously. Aspen Plus assumes you entered the numeric value you intend to use and that you will specify appropriate units for the value.

Defining Your Own Units Set

To define your own units set:

1. From the Data menu, click Setup.
2. In the left pane of the Data Browser, select the Units Sets form.
3. On the Units-Sets Object Manager, click New.
4. In the Create dialog box, enter an ID or accept the default ID for the units set and click OK.

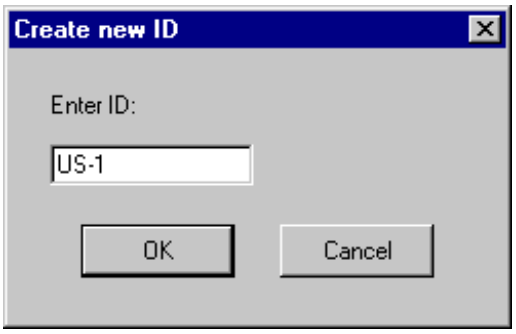
   The unit types you can specify are on six sheets: Standard, Heat, Transport, Concentration, Size, and Miscellaneous.
5. On the Standard sheet, use the drop down arrow in the Copy From/View box to select an existing units set as the starting point for your new units set. Choose the units set that is closest to the new set you are creating.

   Aspen Plus fills in the units for each units type and a dialog box appears.
6. Click Yes or No.
7. If you select Yes, the global units of measurement for both Input data and Output results are changed to the new units set.
8. Click the appropriate sheet and go to the units type you want to modify. Use the drop down arrow to select the units option you want.
9. Repeat Step 6 for all units types you want to modify.

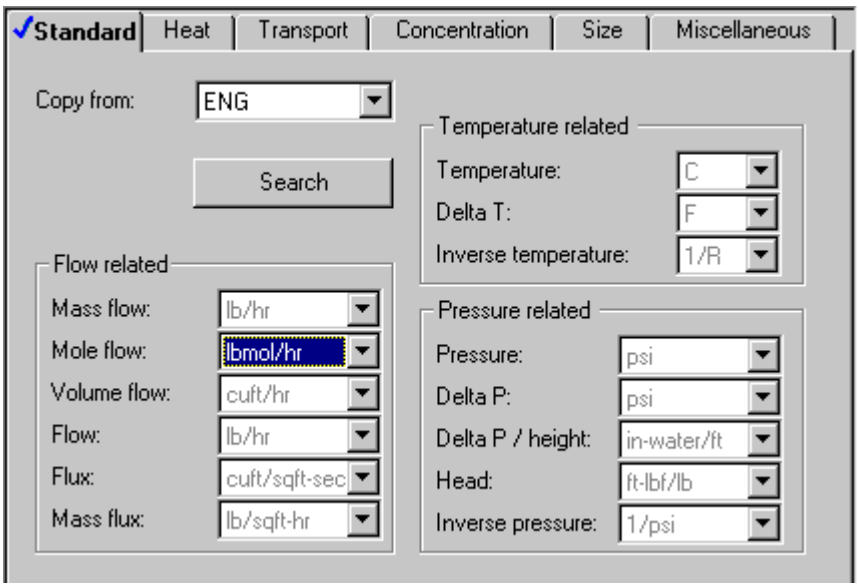
Tip To see all of the units types arranged alphabetically click the Search button.

Example of Defining a New Units Set

1. Create a new units set, US-1, that is identical to the ENG units set, except US-1 uses units of ATM for pressure and C for temperature.
2. From the Data menu, click Setup.
3. In the left pane of the Data Browser, click the Units Sets form.
4. In the Units-Sets Object Manager that appears, click the New button.



5. Accept the default ID in the Create New ID dialog box (US-1).
6. Click OK. The Units-Sets Form appears with the Standard sheet displayed.
7. Aspen Plus asks if you want to make your new units set the global default for subsequent specifications. After you have defined the new units set, you can specify US-1 in the Units box in the Data Browser toolbar.
8. On the Copy From box, use the drop down arrow and select ENG as the set to copy from. The ENG units set values appear in the units box.



9. On the Temperature box, use the drop down arrow and select C as the temperature.
10. On the Pressure box, use the drop down arrow and select atm as the pressure.

Report Options

Use the Setup Report Options form to customize the simulation report. See Chapter 12, for more information on generating and accessing the reports.

Click one of the following for help on customizing the stream report:

- Options for customizing the stream report
- Specifying stream results format
- Including streams
- Designating property sets
- Using the Batch Operation button
- About Batch stream reports
- About Supplementary stream reports

The following table shows what you can specify and where it is located:

On this sheet	Specify
Stream	What stream information is included and in what format. You can use the Standard form to tailor the Stream-Summary report. Use the Batch Operation button to select options for batch streams Items that can be included in the stream report are any combination of Mole, Mass, or Standard Liquid Volume flow or fraction, any number of property sets, component attributes, substream attributes, particle size distribution size limits and stream structure information. Streams can be listed alphanumerically or in the order that they are listed on the flowsheet form. These options are only available when the Stream option is checked on the General sheet.
Property	The property information to be included Items that can be included are List of component IDs, formulas and names, the values in SI units of all physical property parameters used in the simulation, property constant estimation results, and the values of all physical property parameters along with the property parameters' descriptions, equations and sources of data. Additional property files [DMS format input file (*.DFM), Project data file (*.PRJ), and/or Property data format file (*.PRD)] can also be generated automatically when you export a report file. All of these options are only available when the Property option is checked on the General sheet.
ADA	What assay data analysis information is included Items that can be included are the list of generated pseudocomponents, a distillation curve report, and the values of all pseudocomponent property parameters in SI units. All of these options are only available when the ADA option is checked on the General sheet.

Customizing the Stream Report

You can customize the stream format using these options:

Stream Report Options	Description
Flow basis	Display flow rate of each component in each streams in the basis specified. Any combination of Mole, Mass, or Standard Liquid Volume can be chosen.
Fraction basis	Display fraction of each components in each streams in the basis specified. Any combination of Mole, Mass, or Standard Liquid Volume can be chosen.
TFF	Table Format File used to specify the order and format of values printed in the stream report. For more information, see Specifying Stream Results Format on page 5-21.
Report width	Print five streams (80 column) or ten streams (132 column) across a page. Applies only to Report file.
Sort stream alphanumerically	Streams sorted alphanumerically. Applies only to Report file.
Include components with zero flow or fraction	Include components in the stream report, even if they have zero flow or fraction. If this option is not selected, components with zero flow or fraction are not printed for that stream
Include Streams	Specify which streams are printed in the report and order the streams. Applies to the Report file and does not apply to the Stream Results Summary.
Property Sets	Specify property sets for additional properties to be calculated and printed for all of the streams.
Component Attributes	Component attributes, particle size distribution values, particle size distribution size limits and stream structure information can be printed for all of the streams. Applies to the Report file and does not apply to the Stream Results Summary.
Batch Operations	Designated streams can be reported on a batch basis. For more information, see Specifying Batch Streams on page 5-23.
Supplementary stream	Specify additional (supplementary) stream reports. A supplementary report can have different options from the standard report. A supplementary stream report can be generated even if you suppress the standard stream report. Applies to the Report file and does not apply to the Stream Results Summary.

Specifying Stream Results Format

The table format file (TFF) determines the format (order, labels, precision, and other options) of the stream results shown on the Stream Summary sheet.

Aspen Plus provides built-in TFFs tailored to each Application Type, and chooses an appropriate TFF for the Application Type you choose when you create a new run. You can also create your own TFFs. For more information on this, see Chapter 36.

You can specify the TFF in either of these places:

- Format box of the Results Summary Streams Material sheet
- Stream Format box on Setup ReportOptions Stream sheet

Aspen Plus uses the TFF you select in either box for all Results Summary Streams Material sheets you display, until you select another TFF.

It is not necessary to re-run the simulation in order to see the results in another format.

Including Streams

By default, all of the streams are included in the report.

To customize the list of streams to be included in the report:

1. Click the Include Streams button Setup ReportOptions Stream sheet.
2. The right arrow button can be used to move streams from the Available streams list to the Selected streams list to be included in the report. The left arrow button is used to remove streams from the Selected streams list. The double arrows are used to move all of the streams in a list at once.

Designating Property Sets

In addition, you may designate property set IDs for additional stream properties to be included in the report.

To customize the list of property sets to be included in the report:

1. Click the Property Sets button on the Setup ReportOptions Stream sheet.
2. The right arrow button can be used to move Property Sets from the Available property sets list to the Selected property sets list to be included in the report. The left arrow button is used to remove property sets from the Selected property sets list. The double arrows are used to move all of the property sets in a list at once.

Component Attributes

Use the Component Attribute button to select options for component attributes.

Any combination of the following can be printed for all of the streams:

- Component attributes
- Substream attributes
- Particle size distribution (PSD) values
- Particle size distribution size limits
- Stream structure information

Specifying Batch Streams

Use the Batch Operation button to select options for batch streams. The Batch-Operation form is used to designate streams as batch streams and to specify:

- Cycle times
- Down times
- Operation times
- Number of parallel trains for these streams

You can specify just cycle time or any two of the three times.

An Aspen Plus simulation computes the average flow of all streams, assuming continuous steady-state flows. You can designate any type of stream (material, heat, or work) as a batch stream, to report it on a batch basis. Batch stream reporting is used to represent:

- Batch charges
- Batch discharges
- Semi-continuous streams (streams that operate for only a portion of a complete batch cycle)

Each batch stream can have different time specifications, such as cycle time or down time.

All batch stream results appear in the standard stream report of the Aspen Plus report file. The following information is reported:

- Cycle time
- Operation time
- Number of trains
- All material and energy flows in three ways:
  - Average flow rate over entire cycle for all trains
  - Total amount of material and energy per cycle per parallel production train (average flow rate * cycle time / number of trains)
  - Flow rate per train during actual operation
    [amount / cycle / train / operation time]

The Stream Results Summary sheet displays all batch stream results if you select the FULL Table Format File (TFF) on the Format box. If you select PHARM-E, PHARM-M, SPEC-E, or SPEC-M in the Format box, Aspen Plus excludes the operating time, number of trains, and flowrate during actual operation from the stream summary. If you select any other built-in TFF, the stream summary form displays average flow rate of material and energy only. It does not display batch stream results.

To designate a stream as a batch stream:

1. Click the Batch Operation button on the Setup ReportOptions Streams sheet.
2. In the stream box, select a stream ID from the list.
3. You can specify cycle time only, or two of the following times:
   - Cycle time
   - Down time
   - Operation time (Zero indicates an instantaneous charge or discharge.)
4. You can also specify the number of parallel trains. The default is one.

About Supplementary Stream Reports

A supplementary stream report can be generated in the Report file. This selection only applies to the Report file and does not affect to the Stream Results Summary in the graphical user interface.

You can print the standard stream report whether a supplementary stream report is to be generated or not. A supplementary stream report can be generated even if you suppress the standard stream report.

The options available for the Standard stream report are also available for the Supplementary stream report. In addition, a subroutine can be used to generate a user stream report. The subroutine is specified by clicking on the Subroutine button.

6 Specifying Components

This chapter explains how to define the components in your simulation and includes information on:

- Forms for specifying component information
- Specifying databank and non-databank components
- Adding, deleting, and changing components
- Generating electrolyte components and reactions
- Identifying solid components
- Assigning attributes for conventional and nonconventional components
- Specifying supercritical (HENRY) components
- Specifying UNIFAC groups
- Defining component groups

Use these forms to specify component information:

Form	Sheet	What is Specified
Specifications	Selection Petroleum Nonconventional Databanks	All components used in a simulation Assays, blends, and pseudocomponents Nonconventional components Pure component databanks to search for property parameters
Assay/Blend Petro characterization	-	Assays and blends. For more details, see Chapter 32. Pseudo component characterization. For more details, see Chapter 32.
Pseudocomponents		Pseudocomponents data. For more details, see Chapter 32.
Attr-Comps	Selection	Component attributes assigned to conventional components
Henry Components	Selection	Sets of supercritical components for which Henry's law is used in activity coefficient property methods
UNIFAC Groups	Selection	UNIFAC functional groups
Comp-Group	-	Groups of components considered as a unit for tear stream convergence

About Databanks

Aspen Plus stores physical property parameters for a large number of components in several databanks. In addition to the standard Aspen Plus databanks, in-house databanks may be available at your site.

To see the available pure component databanks, and to see or change which databanks are active for a simulation:

1. From the Data menu, click Components.
2. On the Specifications form, click the Databanks sheet.
3. Aspen Plus searches the databanks in the order listed in the Selected Databanks list on this sheet. The default order is appropriate for most simulations.

   To change the search order for databanks in this simulation, click a databank in the Selected Databanks list, and then click the up and down arrow keys to move the databank higher or lower in the list.

   Click here for information about changing search order globally.
4. You can choose additional databanks from the Available Databanks list and add them to the Selected Databanks list using the right arrow button.

   To remove a databank from the search, in the Selected Databanks list, click a databank then click the left arrow button to move it to the Available Databanks list.

This table shows the contents and use of the pure component databanks included with Aspen Plus:

Databank	Contents	Use
PURE10	Pure component parameters for mostly organic components	Primary component databank in Aspen Plus
AQUEOUS	Pure component parameters for ionic and molecular species in aqueous solution	Simulations containing electrolytes
SOLIDS	Pure component parameters for strong electrolytes, salts, and other solids	Simulations containing electrolytes and solids
INORGANIC	Pure component parameters for inorganic and organic components	Solids, electrolytes, and metallurgy applications

Continued

Databank	Contents	Use
PURE856	Version of main pure component databank delivered with Aspen Plus Release 8.5-6	For upward compatibility with previous releases of Aspen Plus
PURE93	Version of main pure component databank delivered with Aspen Plus Release 9.3	For upward compatibility with previous releases of Aspen Plus
AQU92	Version of AQUEOUS delivered with Aspen Plus Release 9.2	For upward compatibility with previous releases of Aspen Plus
ASPENPCD	Version of main pure components databank delivered with Aspen Plus Release 8.5-6	For upward compatibility with previous releases of Aspen Plus.
COMBUST	Pure component parameters for combustion products, including free radicals	For high temperature, gas phase calculations

For information on customizing the default order of the databanks, see Chapter 16.

Specifying Components from a Databank

You must:

- Ensure your simulation contains at least one component.
- Provide Aspen Plus with a list of all the components in the simulation
- Assign a component ID to each component. This ID will refer to the component on all subsequent input forms, results forms, and reports.

To specify the components:

1. From the Data menu, click Components.
2. In the Component ID box of the Selection sheet, type an ID for the component you want to add. Every component must have a Component ID.

Exact match found in databank?	Then Aspen Plus
Yes	Fills in the Formula and Component name. Omit the remaining steps. If you choose not to retrieve data, delete the formula or component name with the backspace key.
No	Requires you to enter the formula or component name, if you want to retrieve data from the databank. To specify the Formula or Component Name yourself, go to Step 3. To use Find, click the Find button and go to Step 4.

3. This table shows what happens:

If you enter a	And an exact match is	Then Aspen Plus
Formula	Found	Fills in the Component Name. You need to specify the Component ID if it has not already been done. Omit the remaining steps.
Formula	Not found	Displays the Find dialog box with any partial match results displayed. See Step 4 for using the Find dialog box. Omit the remaining steps.
Component name	Found	Fills in the Formula. You need to specify the Component ID if it has not already been done.
Component name	Not found	Displays the Find dialog box with any partial match results displayed. See Step 4 for using the Find dialog box.

4. Use the Find dialog box to enter search criteria for your component.

   On the Name or Formula sheet, you can search for strings contained in the name or formula of a component. Using the Advanced sheet, any combination of these items can be entered and used to search for a component:

If you enter a	Then Aspen Plus searches for
Component name or formula	Any components that include the string in any part of the component name or formula
Match only components beginning with this string	Any components that include the string in the beginning of the component name or formula
Component class	A component that is in the component class category
Molecular weight	Components in that molecular weight range
Boiling Point	Components in that boiling point range
CAS number	Component with that Chemical Abstracts Service registry number

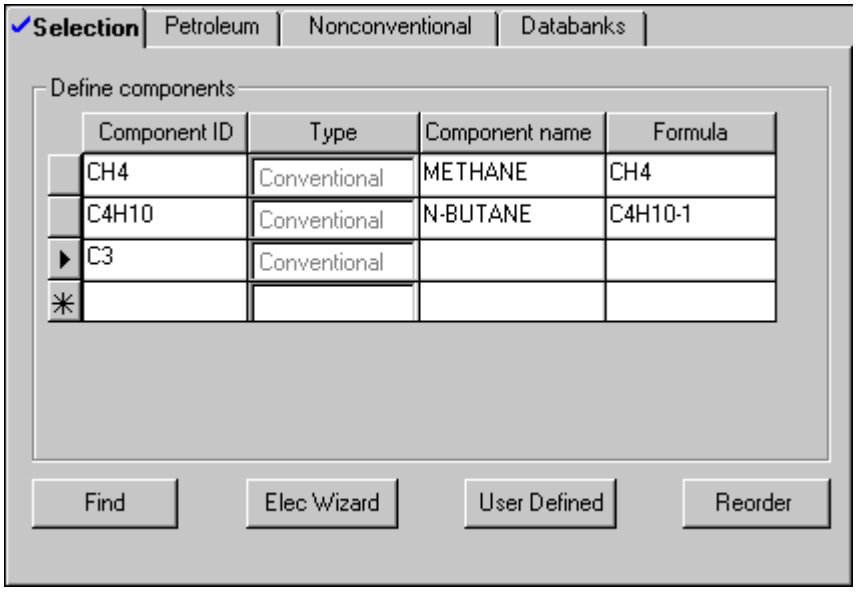
5. Click the Find Now button to display all of the components with your find criteria. Then, select a component from the list and click Add to add it to the components list. Click here to see an example of using Find.
6. When you finish searching for components, click Close to return to the Selection sheet.

You can return to the Components Specifications Selection sheet at any time while building your simulation, to add or delete components.

If you enter a	Then Aspen Plus searches for
Component name or formula	Any components that include the string in any part of the component name or formula.
Match only components beginning with this string	Any components that include the string in the beginning of the component name or formula.
Component class	A component that is in the component class category.
Molecular weight	Components in that molecular weight range.
Boiling Point	Components in that boiling point range.
CAS number	Components with that Chemical Abstracts Service registry number.

Example of Specifying Components

In this example, the Formula and Component Name for component CH4 are automatically retrieved from the databanks. Data for components CH4 and C4H10 is retrieved from the databanks. Component C3 is a non-databank component.



Example of Using the Find Dialog Box

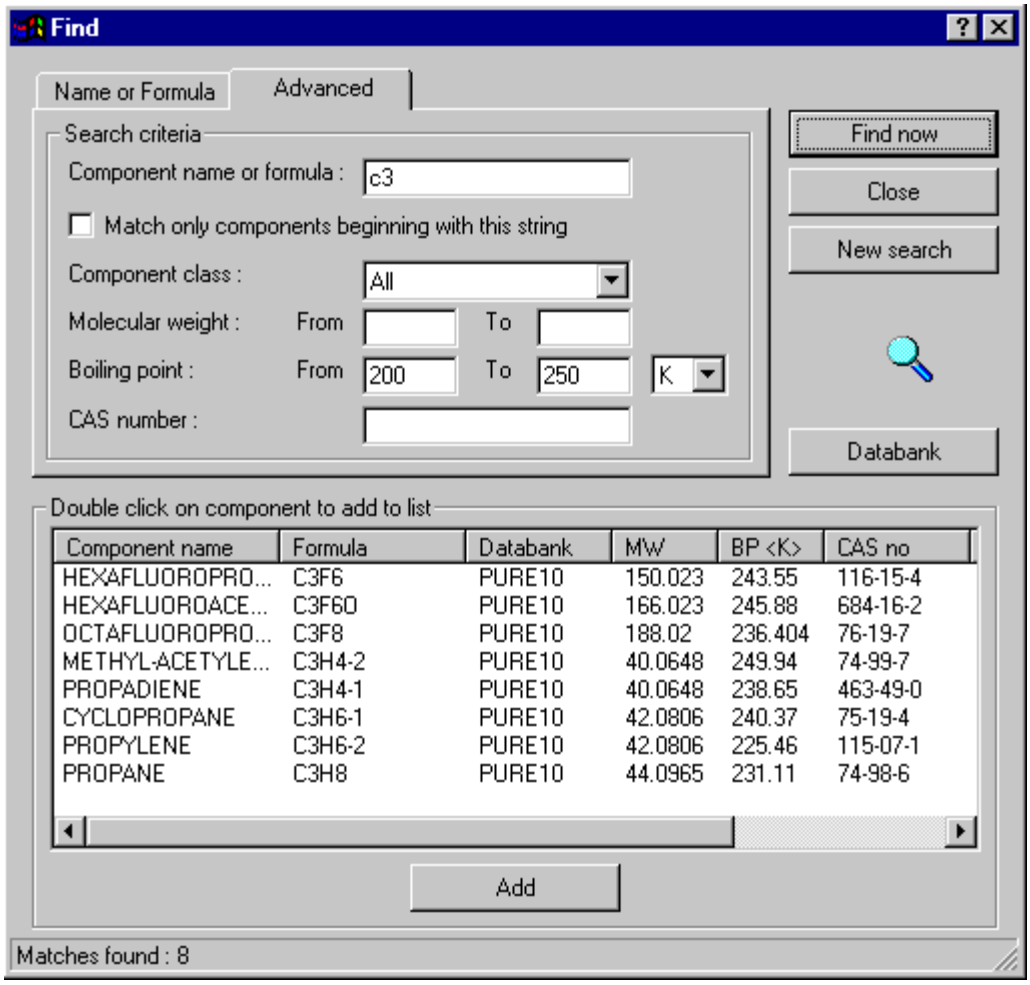
In this example, the advanced component Find dialog box is used to locate a component that includes C3 in its formula and has a boiling point between 200 and 250 K.

To do this:

1. On the Components Specifications Selection sheet, select an empty component ID field, then click Find.
2. In the Component Name or Formula box, enter C3.
3. Select the Advanced sheet where you can also search for components based on the chemical class, molecular weight range, boiling point range and CAS number.
4. In the Boiling Point boxes, enter from 200 to 250 K.
5. Click Find Now.

   Aspen Plus searches its databanks for components that contain the characters C3 in the name or formula and have a Boiling point between 200 and 250 K and then displays the results in the bottom half of the window.
6. To include a component from the search results in your simulation, select a component name from the list, and click Add. From the Find dialog box, you can continue to select component names and click the Add button to select multiple components from the search results to be added to your simulation. You can also modify your search criteria and click Find Now again to generate new search results.
7. When finished, click Close to return to the Components Specifications Selection sheet.

   Click here to see the Find dialog box for this example.



Specifying Non-Databank Components

To define a component that is not in the databanks:

1. From the Data menu, click Components.
2. On the Specifications Selection sheet, enter only the Component ID.
3. If Aspen Plus finds a match in a databank for the ID you enter, delete the Formula or Component Name. Aspen Plus then recognizes the component as a non-databank component.
4. You must supply all required property parameters for non-databank components. You can supply the parameters yourself using the Properties Data and Parameters forms.

– or –

Combine user-input parameters and data with one or both of the following:

- Property Estimation to estimate the required parameters using the Properties Estimation forms
- Data Regression to regress data to obtain the parameters using the Properties Regression forms

For information on	See
Physical property data requirements	Chapter 8
Estimating property parameters	Chapter 30
Regressing property parameters	Chapter 31

Tip Use the User Defined Component Wizard to help you enter some of the commonly available data, such as normal boiling point and vapor pressure data.

Using the User Defined Component Wizard

You can use the User Defined Component Wizard to define the properties needed for conventional, solid, and nonconventional components. You can modify the parameters supplied at any time by returning to the User Defined Component Wizard or by going to the forms where the information is saved.

Use this wizard to define components that are not in any pure component databanks. You can define conventional components, solid components, and nonconventional components. The wizard also helps you enter commonly available data for the components, such as molecular weight, normal boiling point, vapor pressure and heat capacity data.

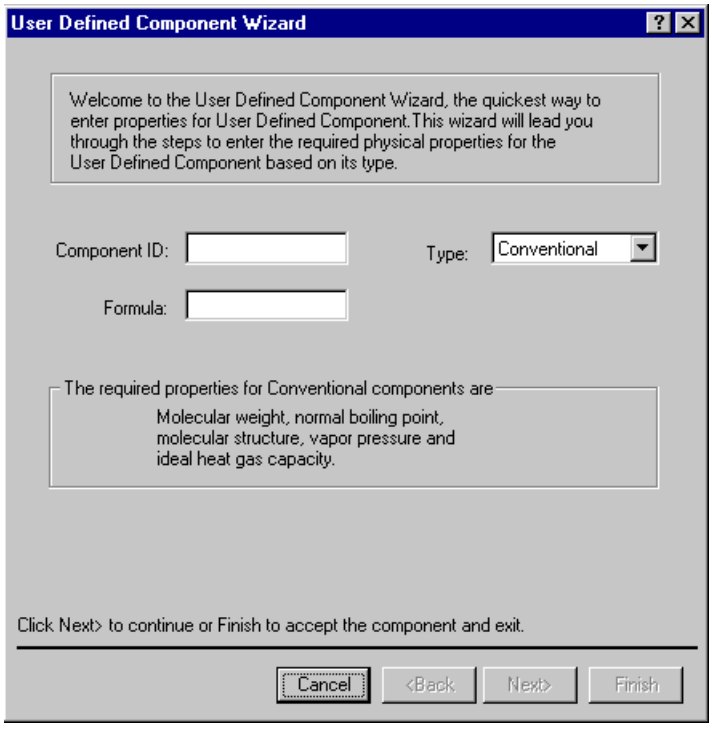
Tip You can also select a databank on the Components Specifications Selection sheet and give it a different chemical formula. This special formula can be used to identify the component in user-written subroutines. This allows property parameters for the component to be retrieved from the databanks.

To open the User Defined Component Wizard:

1. From the Data menu, click Components.
2. On the Specifications Selection sheet, click the User Defined button.

   The User Defined Component Wizard appears.

Tip For help on the wizard, click the What's This button in the right hand corner of the wizard dialog box, then click any part of the wizard.



Defining a Conventional Component

To define a conventional component, open the user defined component wizard then:

1. Enter the Component ID. Every component in the flowsheet must have a Component ID. This ID is used to refer to the component throughout the simulation.
2. From the Type list, click Conventional.
3. Optionally, enter a formula for the component. The formula can identify the component in user-written property or unit operation model subroutines. If the formula for the component exists in an Aspen Plus databank, a warning message appears.
4. Click Next.
5. Enter the molecular weight and normal boiling point in the respective boxes on the Conventional Components Basic Data dialog box.

   The molecular structure, molecular weight, and normal boiling point are the most fundamental information required in group-contribution and corresponding-states methods used in property estimation.

Molecular weight is required in all simulations. If the Molecular structure is later entered, the molecular weight used in the simulation can be calculated from the atoms.

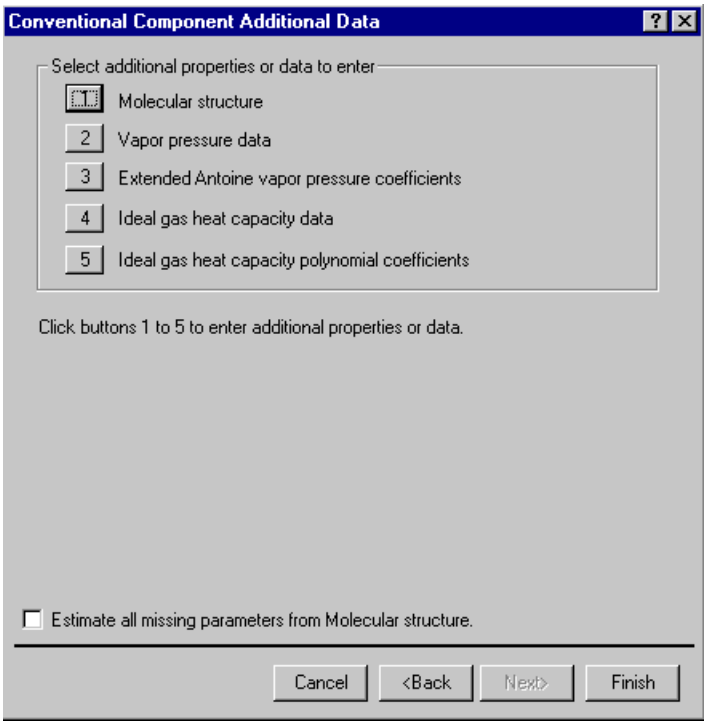
Normal boiling point is not required per se in property calculations, but is used to estimate many other parameters such as critical temperature and critical pressure, if they are missing.

6. Optionally enter the data shown in the following table. This data can be found later on the Properties Parameters Pure Component USRDEF-1 form.

Physical Property	Information
Specific gravity at 60°F (SG)	
Standard enthalpy of formation (DHFORM)	Most simulations involve energy balance calculations therefore enthalpy is required. Standard enthalpy of formation of ideal gas at 25°C (DHFORM) is used in the enthalpy calculation, but is not required unless the simulation contains chemical reactions, because DHFORM defaults to zero.
Standard Gibbs energy of formation (DGFORM)	Enter the standard Gibbs energy of formation of ideal gas at 25°C (DGFORM) if either: • The simulation contains chemical reactions. • You use the RGibbs unit operation model.

7. If you wish to enter additional property information, such as molecular structure, vapor pressure or ideal gas heat capacity data, click Next. The wizard will help you enter property data, property parameters, and molecular structure or activate property estimation.

8. If you clicked Next to enter additional property data, this dialog box appears:



9. Click the buttons to enter additional properties or data.

This table provides information about the properties or data:

Type	Description
Molecular structure	Component Molecular Structure Molecular structure is required in all group-contribution methods used to estimate missing property parameters. If you enter molecular structure, you should also request estimation of parameters by selecting the Estimate All Missing Parameters From Molecular Structure check box. The structure can be modified later if needed, on the Properties Molecular Structure form. For details on entering molecular structure or Property Estimation, see Chapter 30.
Vapor pressure data	Vapor pressure data used to determine extended Antoine vapor pressure coefficients (PLXANT) from Property Estimation using the Data method. If you enter vapor pressure data, you should also request estimation of parameters by selecting the Estimate All Missing Parameters From Molecular Structure check box. The data you enter can be modified later on the Properties Data form with the name you defined. The data can also be used with Data Regression. For information on entering pure component data or Data Regression, see Chapter 31.

Continued

Type	Description
Extended Antoine vapor pressure coefficients	Coefficients for the extended Antoine vapor pressure equation (PLXANT) These parameters can be modified later on the Properties Parameters Pure Components PLXANT-1 form. For more information on entering or modifying property parameters, see Chapter 8.
Ideal gas heat capacity data	Ideal gas heat capacity data used to determine coefficients for the ideal gas heat capacity equation (CPIG) from Property Estimation using the Data method. (For more information see Chapter 30.) If you enter Ideal gas heat capacity data, you should also request estimation of parameters by selecting the Estimate All Missing Parameters From Molecular Structure check box. The data you enter can be modified later on the Properties Data form with the name you defined. The data can also be used with Data Regression. For information on Data Regression, or entering pure component data, see Chapter 31.
Ideal gas heat capacity polynomial coefficients	Coefficients for the ideal gas heat capacity equation (CPIG) These parameters can be modified later on the Properties Parameters Pure Components CPIG-1 form. For more information on entering or modifying property parameters, see Chapter 8.

10. Optionally, select the Estimate All Missing Parameters From Molecular Structure check box.
11. Click Finish to close the wizard and return to the Components Specifications Selection sheet.

Defining a Solid Component

The steps used to define a solid component are almost the same as those for conventional components. You must select Solid from the Type list in Step 2 above, and the types of data or parameters you can enter are pertinent to solid components.

Normal boiling point is not required per se in property calculations, but is used to estimate many other parameters such as critical temperature and critical pressure if they are missing. If you have an experimental normal boiling point, you should enter it.

Since most simulations involve energy balance calculations, enthalpy is required. Solid enthalpy of formation of solids (DHSFRM) is used in the enthalpy calculations, but is not required unless the simulation contains chemical reactions, because DHSFRM defaults to zero.

Defining a Nonconventional Component

To define a nonconventional component, open the User Defined Component wizard, then:

1. Enter the Component ID. Every component in the flowsheet must have a Component ID. This ID is used to refer to the component throughout the simulation.
2. Select Nonconventional from the Type list.
3. Click Next.
4. Choose Enthalpy and Density models by selecting from the Enthalpy and Density lists respectively. The required component attributes for the selected models are shown below the model selections.

   For more information on properties for nonconventional components, see Chapter 7.
5. Click Finish to close the wizard and return to the Components Specifications Selection sheet.

   The nonconventional property specifications you entered are saved under the Properties Advanced NC-Props form.

Adding a Component

To add a component to the existing component list:

1. From the Data menu, click Components.
2. On the Specifications Selection sheet, move to the first blank row.
3. Enter a Component ID, name or formula.

   Follow the next two steps if you wish to move the component within the list.
4. Click the Reorder button to open the Reorder Components dialog box.
5. Select the new component and move it up in the sequence with the up arrow to the right of the components list.

Inserting a Component

To insert a component:

1. From the Data menu, click Components.
2. On the Specifications Selection sheet, move to the row where you want the new component inserted.
3. Click the right mouse button and from the menu that appears, click Insert Row.
4. Enter a Component ID, name or formula in the new row.

Renaming a Component

To rename an existing component:

1. From the Data menu, click Components.
2. On the Specifications Selection sheet, move to the Component ID box for the component you want to rename.
3. Type over the existing ID.

   Aspen Plus prompts you to either delete or rename the existing component.
4. Select Rename.

The component is renamed on this form and on all other forms where it appears. No data is lost.

If you select Delete, both the Component ID and its data is deleted.

Deleting a Component

To delete a component:

1. From the Data menu, click Components.
2. On the Specifications Selection sheet, click the right mouse button on the row selector for the component you want to delete.
3. Choose Delete Row from the menu that appears.

   When you delete a component, all references to the component on other sheets are automatically deleted. For example, if you entered component flows on a Stream form, then you deleted a component on the Components Specifications Selection sheet. Aspen Plus automatically deletes the component ID and flow from the Stream form.

Reordering the Component List

To reorder the list of components on the Components Specifications Selection sheet:

1. From the Data menu, click Components.
2. On the Specifications Selection sheet, click the Reorder button.
3. Click the ID of the component you wish to move.
4. Move the component in the appropriate direction, by clicking the up or down arrows to the right of the list.
5. Repeat Steps 3 and 4 until all components are ordered as desired.
6. Click Close to return to the Specifications Selection sheet which displays the components with the new order.

   Aspen Plus retains all original data and references for the components on this and other forms.

Generating Electrolyte Components and Reactions

Electrolyte systems involve ionic components and reactions that must be defined to complete the components specification. You can use the Electrolyte Wizard to generate ionic reactions and additional components that might be formed by the reactions.

Before opening the Electrolyte Wizard:

1. From the Data menu, click Components.
2. On the Specifications Selection sheet, enter the component Water (H2O). Electrolyte systems must have water present.
3. Enter the additional molecular components that define the system. Some examples are:

System	Molecular Components
Sour water system	CO2, H2S, O2S (for SO2)
Brine system	NACL (use Type = Conventional, do not identifyType as Solid)

4. Click the Elec Wizard button.
5. On the Electrolytes Wizard dialog box, click Next.

Tip For Help on the Wizard click the What's This button in the wizard and then click any active field in the Wizard.

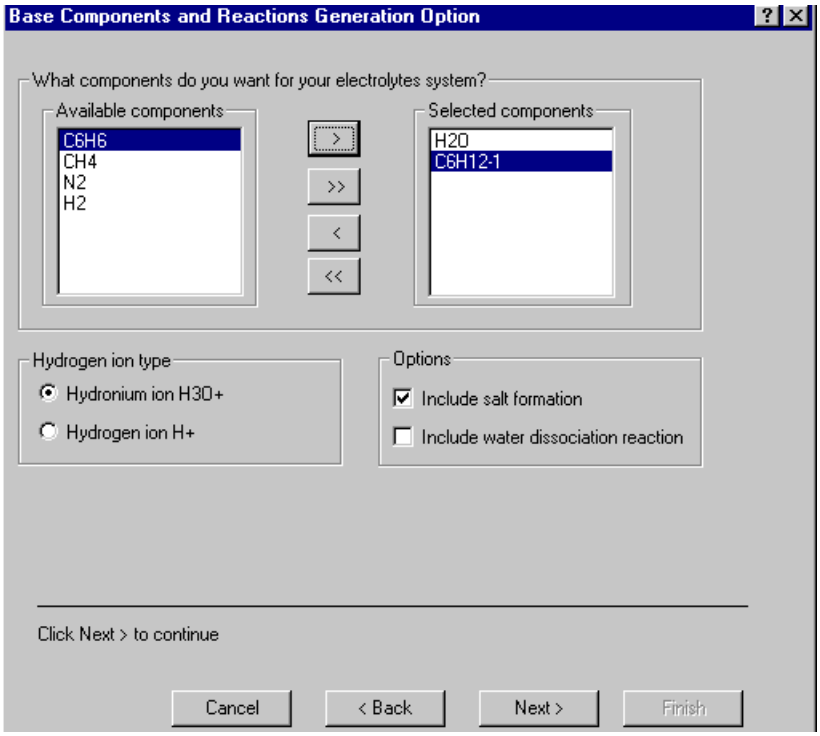
Generating the List of Components

To generate the list of required components:

1. From the left pane of the Data Browser, double-click the Components folder, then click Specifications.
2. On the Selection form, click the Elec Wizard button.
3. Click Next on the first Electrolyte wizard dialog box that appears.
4. On the Base Components and Reactions Generation Option dialog box, select the components from which you want to generate reactions and ionic species.

5. To move an individual component from the Available Components list, click an individual component and then click the single right arrow.

   To move all components to the Selected components list, click the double arrow.



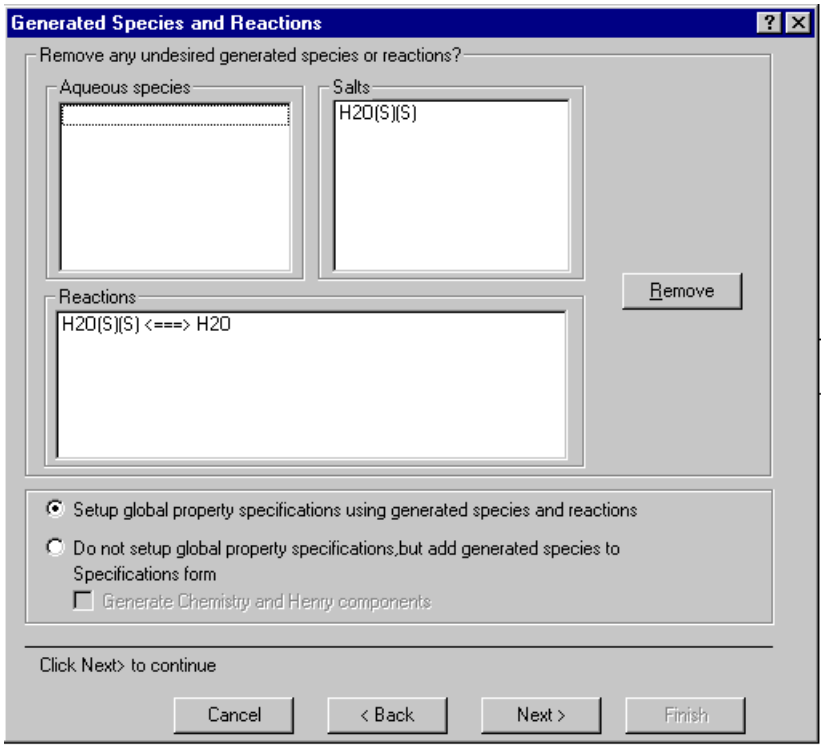
6. Turn the other options on or off to match your preferences.

   The recommended hydrogen ion type is Hydronium ion H3O+. You may toggle this to use Hydrogen ion H+.

Select this option	To
Include Salt Formation	Include solid salts when new species are generated. Default (On) is to include salts.
Include Water Dissociation Reaction	Include water dissociation in the list of generated reactions. Default (Off) is not to include water dissociation reaction.

7. Click Next.

   On the Generated Species and Reactions dialog box, Aspen Plus displays lists of aqueous species, salts, and reactions.



For reactions, arrows pointing in both directions mean ionic equilibrium or salt precipitation. An arrow pointing in one direction means complete dissociation. Generated solid salt components are assigned component IDs with (S) to indicate the solid type.

8. Remove any unwanted items by selecting them and clicking Remove. Removing any species will remove all reactions containing that species.
9. Click Next.
10. On the Simulation Approach dialog box, choose the simulation approach.

Choose this approach	To have	The Calculation method is
True †	All calculated results displayed in terms of the actual species present (molecular, ionic, and solid forms of the same electrolyte will each be shown separately).	Electrolyte reactions solved simultaneously with phase equilibrium equations in unit operation models
Apparent	All forms of the same electrolyte show up as a single component	Electrolyte reactions solved during property evaluations

† *The default true component approach is generally preferred for calculation efficiency.*

Both approaches give the same results. You are also shown the name of the Chemistry ID (GLOBAL) and the Henry-Comps ID (also GLOBAL).

11. Click Next to create the Chemistry and Henry-Comps forms and go on to the Summary sheet.

The Summary dialog box summarizes the modifications made by the Electrolyte Wizard to your properties, components, databanks, and chemistry specifications. Review or modify the generated specifications for Henry components or for electrolyte reactions on the Summary dialog box.

Reviewing Generated Henry Components

To review or modify the Henry Components list generated by the Electrolytes Wizard:

1. Click the Review Generated Henry-Comps List button on the Summary dialog box.
2. On the Henry Components Global dialog box, select components and use the right and left arrow buttons to add or remove from the Selected Components list.
3. Click the X in the upper right corner of the dialog box when finished to close the dialog box.
4. Note that Henry component specifications can be modified later using the Components Henry-Comps forms.

Reviewing Generated Electrolyte Reactions

To review or modify the electrolyte reactions generated by the Electrolyte Wizard:

1. Click the Modify/Add Reactions button on the Summary dialog box.
2. On the Modify/Add Reactions Global dialog box, the Stoichiometry sheet displays the reactions, their type, and their stoichiometry. To modify reaction stoichiometry for a reaction, select it from the list, and click Edit. When you finish modifying the stoichiometry, click Close.
3. Use the Equilibrium Constants sheet to enter, review, or change the Equilibrium constants, their concentration basis, or the temperature approach to equilibrium. To view or modify equilibrium constant information for other reactions, select the desired reaction from the Equilibrium Reaction list.
4. Click the X in the upper right corner of the dialog box when finished.

   Electrolyte chemistry specifications can be modified later using the Reactions Chemistry forms.

   After reviewing the information on the Summary dialog box, click Finish to save all the changes to the appropriate forms and to return to the Components Specifications Selection sheet.

For more information about modeling your process with electrolytes, see *Aspen Plus Physical Property Methods and Models* or the Getting Started guide.

Identifying Solid Components

To identify components as solids:

1. From the Data menu, click Components.
2. On the Specifications Selection sheet, specify the Component ID.
3. If the component is a databank component, specify the formula and component name. For more information, see Specifying Components from a Databank on page 6-1.
4. In the Type box, specify Solid for a conventional solid or Nonconventional for a nonconventional solid.

Conventional Solids

Conventional solids are pure materials. These solids may be present in mixtures in phase and/or chemical equilibrium, including electrolyte salts. For example, NaCl can be a conventional solid precipitating from an electrolyte solution. These solids are present in the MIXED substream.

Conventional solids are characterized in terms of properties, such as:

- Molecular weight
- Vapor pressure
- Critical properties

Conventional solids that do not participate in phase equilibrium calculations are conventional inert solids. Conventional inert solids:

- Can participate in chemical equilibrium, modeled by the RGibbs unit operation model. None of the other unit operation models handles solid equilibrium.
- Are assigned the substream type CISOLID to distinguish them from other conventional solids

Nonconventional Solids

Nonconventional solids are materials characterized in terms of empirical factors called component attributes. Component attributes represent component composition by one or more constituents.

Nonconventional solids never participate in phase or chemical equilibrium calculations. Aspen Plus always assigns substreams of type NC to nonconventional solids.

Examples of nonconventional solids are coal and wood pulp.

About Component Attributes

Component attributes represent component composition in terms of one or more sets of constituents. For example, coal is often characterized in terms of ultimate and proximate analyses, as well as several other types of analysis.

You can assign component attributes to non-solid conventional components (Type is Conventional).

The standard Aspen Plus property models and unit operation models do not use these attributes in any calculations. But assigning attributes lets you keep track of properties that do not affect material and energy balance calculations. For example, you could assign component attributes to account for the color or odor of a component. You can use component attributes in Fortran subroutines for property models or unit operation calculations that you write.

The following table describes available component attributes:

Component Attribute	Description	Elements
PROXANAL	Proximate analysis, weight %	1 Moisture (moisture-included basis) 2 Fixed carbon (dry basis) 3 Volatile Matter (dry basis) 4 Ash (dry basis)
ULTANAL	Ultimate analysis, weight %	1 Ash (dry basis) 2 Carbon (dry basis) 3 Hydrogen (dry basis) 4 Nitrogen (dry basis) 5 Chlorine (dry basis) 6 Sulfur (dry basis) 7 Oxygen (dry basis)

Continued

Component Attribute	Description	Elements
SULFANAL	Forms of sulfur analysis, weight % of original coal	1 Pyritic (dry basis) 2 Sulfate (dry basis) 3 Organic (dry basis)
GENANAL	General constituent analysis, weight %	1 Constituent 1 2 Constituent 2 . . 20 Constituent 20

For information on entering component attribute values in streams, see Chapter 9, Specifying Streams.

Assigning Attributes to Conventional Components

To assign attributes to a conventional or conventional solid component:

1. From the Data menu, click Components.
2. In the left pane of the Data Browser, click Attr-Comps.
3. On the Selection sheet, choose a Component ID from the Component list. You may select more components by listing them below the first one.
4. Select a component attribute from the Attributes list. You may list multiple component attributes for each component.

In most cases, the conventional components to which you assign attributes will be solids (Type is Solid on the Components Specifications Selection sheet).

For information on entering component attribute values in streams, see Chapter 9, Specifying Streams.

Assigning Attributes to Nonconventional Components

Attributes for nonconventional components are automatically assigned when you select nonconventional enthalpy and density models on the Properties Advanced NC-Props form, or use the User Defined Components wizard with a nonconventional component.

You can assign additional component attributes to nonconventional components. To do this:

1. From the Data menu, select Physical Properties.

2. In the left pane of the Data Browser, double-click the Advanced folder.
3. Click NC-Props.
4. Select a component from the Component list.
5. Enter the enthalpy and density model names for that component, if this has not already been done.

   The required component attributes for the selected models will be automatically listed at the bottom of the sheet.
6. Add component attributes to the Required Component Attributes For The Selected Models box by selecting them from the list.

For more information on	See
Property methods for nonconventional components	Chapter 7, Physical Property Methods
Parameters for nonconventional components	Chapter 8, Physical Property Parameters and Data
Entering component attribute values	Chapter 9, Specifying Streams

Specifying Supercritical (HENRY) Components

In the activity-coefficient approach for computing vapor-liquid equilibrium, Henry's law is used to represent the behavior of dissolved gases or other supercritical components.

To use Henry's law in Aspen Plus, you must define one or more sets of supercritical (or Henry's) components.

For Henry's law to be used during property calculations, you must also specify a Henry Components ID on one of these sheets:

- Properties Specifications Global sheet
- Properties Specifications Flowsheet Sections sheet
- A unit operation BlockOptions Properties sheet
- A Property Analysis Properties sheet

Aspen Plus has built-in Henry's law parameters for a large number of component pairs. The solvents are water and other organic compounds.

These parameters are used automatically on the Properties Parameters Binary Interaction HENRY-1 form when you specify a property method that uses Henry Comps. For components that do not have Henry's law parameters available, you must enter Henry's law parameters on the Properties Parameters Binary Interaction HENRY-1 form. See Chapter 8 for a discussion of physical property parameter requirements.

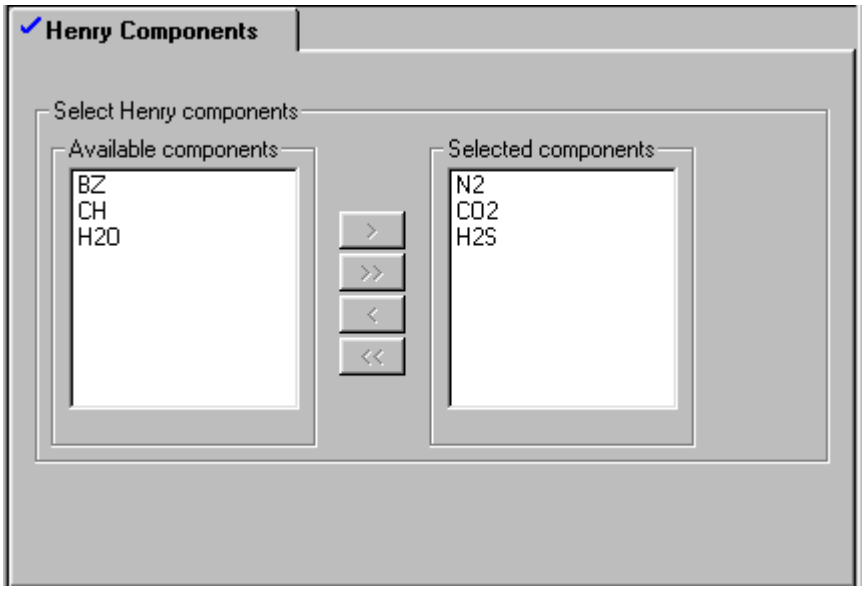
To define a set of Henry's components:

1. From the Data menu, click Components.
2. In the left pane of the Data Browser, click Henry Comps.
3. On the Henry Components Object Manager, click New.
4. In the Create New ID dialog box, enter an ID for a new list of Henry Components, or accept the default ID.
5. Specify the Component IDs in Selected components list.

   Select the components to include as Henry components from the Available components list and use the right arrow button to move them into the Selected components list. The left arrow can be used to remove components from the Selected components list. The double arrow can be used to move all of the components in a list at one time.

Example of Specifying Henry's Components

In this example, N2, CO2, and H2S are identified as Henry's components. BZ, CH, and H2O are not selected as Henry components.



Specifying UNIFAC Groups

Use the Components UNIFAC Groups Selection sheet to identify UNIFAC groups or to introduce new groups. If you want to enter UNIFAC group parameters or group-group interaction parameters, you must assign an ID to each group. Use the group ID on the Properties Parameters UNIFAC Group form or UNIFAC Group Binary form to enter group parameters.

To specify UNIFAC groups:

1. From the Data menu, choose Components.
2. In the left pane of the Data Browser, click UNIFAC Groups.
3. On the UNIFAC Groups Selection sheet, type a name for the group in the Group ID box. Every group needs a name that can be referenced on other forms.
4. Select a number from the Group number list. As you scroll, a brief description of each group appears in the description area.

   If you want to define a new UNIFAC group, type in a number between 4000 and 5000 in the Group number box.

Defining Component Groups

You can specify a group of components to be converged in a tear stream.

A component group consists of either a:

- List of components
- Range of components from the Components Specifications Selection sheet
- Combination of component lists and ranges

To define a component group:

1. From the Data menu, click Components.
2. In the left pane of the Data Browser, click Comp-Group.
3. In the Component Group Object Manager, click New.
4. In the Create New ID dialog box, enter an ID for the new Component Group or accept the default.

   5. On the Component List sheet, choose a substream from the Substream list.

5. Specify the components to be included in the component group.

   Select the components to include from the Available components list and use the right arrow button to move them into the Selected components list. The left arrow can be used to remove components from the Selected components list. The double arrows can be used to move all of the components in a list at one time.

   Alternatively, you can click the Component Range sheet, and enter a range of components that represent your component group.

7. If you want to create a component group containing components from more than one substream, repeat steps 5 and 6.

Using a component group can aid tear stream convergence when you use the NEWTON, BROYDEN, or SQP convergence methods and your flowsheet has all of the following:

- Recycles
- A large number of components
- Some components known to have zero or constant flow rates

A component group reduces the problem matrix size and the number of numerical derivative perturbations (if performed). This makes convergence faster and more stable.

To use a component group for a convergence method, you must specify the Component Group ID in one of the following sheets:

- Convergence Convergence Input Tear Streams sheet
- Convergence Conv-Options Defaults Tear Convergence sheet

7 Physical Property Methods

Choosing the appropriate property method is often the key decision in determining the accuracy of your simulation results. This chapter provides guidelines for choosing appropriate property methods and models including:

- What is a property method
- Available property methods
- Choosing a property method
- Creating new property methods
- Specifying the global property method
- Specifying a property method for a flowsheet section
- Specifying a local property method
- Defining supercritical components
- Specifying properties for the free-water phase
- Special method for K-value of water in the organic phase
- Specifying electrolyte calculations
- Modifying property methods
- Property methods for nonconventional components

What Is a Property Method?

A property method is a collection of methods and models that Aspen Plus uses to compute thermodynamic and transport properties.

The thermodynamic properties are:

- Fugacity coefficient (K-values)
- Enthalpy
- Entropy
- Gibbs free energy
- Volume

The transport properties are:

- Viscosity
- Thermal conductivity
- Diffusion coefficient
- Surface tension

Aspen Plus includes a large number of built-in property methods that are sufficient for most applications. However, you can create new property methods to suit your simulation needs.

Available Property Methods

You must select one or more Property Methods to model the properties of specific systems in your flowsheet. Each property method has a unique approach to representing K-values.

The following tables list all of the property methods available in Aspen Plus.

You can modify these existing methods or create new methods. For more information, see Modifying Property Methods on page 7-18.

Property Methods

Ideal Property Methods

Ideal Property Method	K-Value Method
IDEAL	Ideal Gas/Raoult's law/Henry's law
SYSOP0	Release 8 version of Ideal Gas/Raoult's law

Equation-of-State Property Methods

Equation-of-State Property Method	K-Value Method
BWR-LS	BWR Lee-Starling
LK-PLOCK	Lee-Kesler-Plöcker
PENG-ROB	Peng-Robinson
PR-BM	Peng-Robinson with Boston-Mathias alpha function
PRWS	Peng-Robinson with Wong-Sandler mixing rules
PRMHV2	Peng-Robinson with modified Huron-Vidal mixing rules
PSRK	Predictive Redlich-Kwong-Soave
RKSWS	Redlich-Kwong-Soave with Wong-Sandler mixing rules
RKSMHV2	Redlich-Kwong-Soave with modified Huron-Vidal mixing rules
RK-ASPEN	Redlich-Kwong-ASPEN
RK-SOAVE	Redlich-Kwong-Soave
RKS-BM	Redlich-Kwong-Soave with Boston-Mathias alpha function
SR-POLAR	Schwartzentruber-Renon

Activity Coefficient Property Methods

Activity Coefficient Property Method	Liquid Phase Activity Coefficient Method	Vapor Phase Fugacity Coefficient Method
B-PITZER	Bromley-Pitzer	Redlich-Kwong-Soave
ELECNRTL	Electrolyte NRTL	Redlich-Kwong
ENRTL-HF	Electrolyte NRTL	HF Hexamerization model
ENRTL-HG	Electrolyte NRTL	Redlich-Kwong
NRTL	NRTL	Ideal gas
NRTL-HOC	NRTL	Hayden-O'Connell
NRTL-NTH	NRTL	Nothnagel
NRTL-RK	NRTL	Redlich-Kwong
NRTL-2	NRTL (using dataset 2)	Ideal gas
PITZER	Pitzer	Redlich-Kwong-Soave
PITZ-HG	Pitzer	Redlich-Kwong-Soave
UNIFAC	UNIFAC	Redlich-Kwong
UNIF-DMD	Dortmund-modified UNIFAC	Redlich-Kwong-Soave
UNIF-HOC	UNIFAC	Hayden-O'Connell
UNIF-LBY	Lyngby-modified UNIFAC	Ideal gas
UNIF-LL	UNIFAC for liquid-liquid systems	Redlich-Kwong
UNIQUAC	UNIQUAC	Ideal gas
UNIQ-HOC	UNIQUAC	Hayden-O'Connell
UNIQ-NTH	UNIQUAC	Nothnagel
UNIQ-RK	UNIQUAC	Redlich-Kwong
UNIQ-2	UNIQUAC (using dataset 2)	Ideal gas
VANLAAR	Van Laar	Ideal gas
VANL-HOC	Van Laar	Hayden-O'Connell
VANL-NTH	Van Laar	Nothnagel
VANL-RK	Van Laar	Redlich-Kwong
VANL-2	Van Laar (using dataset 2)	Ideal gas
WILSON	Wilson	Ideal gas
WILS-HOC	Wilson	Hayden-O'Connell
WILS-NTH	Wilson	Nothnagel
WILS-RK	Wilson	Redlich-Kwong
WILS-2	Wilson (using dataset 2)	Ideal gas

Continued

Activity Coefficient Property Method	Liquid Phase Activity Coefficient Method	Vapor Phase Fugacity Coefficient Method
WILS-HF	Wilson	HF Hexamerization model
WILS-GLR	Wilson (ideal gas and liquid enthalpy reference state)	Ideal gas
WILS-LR	Wilson (liquid enthalpy reference state)	Ideal gas
WILS-VOL	Wilson with volume term	Redlich-Kwong

Property Methods for Special Systems

Property Methods for Special Systems	K-Value Method	System
AMINES	Kent-Eisenberg amines model	H2S, CO2, in MEA, DEA, DIPA, DGA solution
APISOUR	API sour water model	Sour water with NH3, H2S, CO2
BK-10	Braun K-10	Petroleum
SOLIDS	Ideal Gas/Raoult's law/Henry's law/solid activity coefficients	Pyrometallurgical
CHAO-SEA	Chao-Seader corresponding states model	Petroleum
GRAYSON	Grayson-Streed corresponding states model	Petroleum
STEAM-TA	ASME steam table correlations	Water/steam
STEAMNBS	NBS/NRC steam table equation of state	Water/steam

Choosing a Property Method

Use the tables starting on page 7-6 and the figures on page 7-10 to select the best property method for your simulation. For more information, see also Chapter 8 for detailed descriptions of the data requirements for each property method. Many methods contain extensive built-in binary parameters, so they are essentially predictive.

Recommended Property Methods for Different Applications

Use these tables as guidelines for selecting the best property method for your simulation.

Oil and Gas Production

Application	Recommended Property Methods
Reservoir systems	PR-BM, RKS-BM
Platform separation	PR-BM, RKS-BM
Transportation of oil and gas by pipeline	PR-BM, RKS-BM

Refinery

Application	Recommended Property Methods
Low pressure applications (up to several atm) Vacuum tower, atmospheric crude tower	BK10, CHAO-SEA, GRAYSON
Medium pressure applications (up to several tens of atm) Coker main fractionator, FCC main fractionator	CHAO-SEA, GRAYSON, PENG-ROB, RK-SOAVE
Hydrogen-rich applications Reformer, Hydrofiner	GRAYSON, PENG-ROB, RK-SOAVE
Lube oil unit, De-asphalting unit	PENG-ROB, RK-SOAVE

Gas Processing

Application	Recommended Property Methods
Hydrocarbon separations Demethanizer C3-splitter	PR-BM, RKS-BM, PENG-ROB, RK-SOAVE
Cryogenic gas processing Air separation	PR-BM, RKS-BM, PENG-ROB, RK-SOAVE
Gas dehydration with glycols	PRWS, RKSWS, PRMHV2, RKSMHV2, PSRK, SR-POLAR
Acid gas absorption with Methanol (RECTISOL) NMP (PURISOL)	PRWS, RKSWS, PRMHV2, RKSMHV2, PSRK, SR-POLAR

Continued

Application	Recommended Property Method
Acid gas absorption with Water Ammonia Amines Amines + methanol (AMISOL) Caustic Lime Hot carbonate	ELECNRTL
Claus process	PRWS, RKSWS, PRMHV2, RKSMHV2, PSRK, SR-POLAR

Petrochemicals

Application	Recommended Property Methods
Ethylene plant Primary fractionator	CHAO-SEA, GRAYSON
Light hydrocarbons Separation train Quench tower	PENG-ROB, RK-SOAVE
Aromatics BTX extraction	WILSON, NRTL, UNIQUAC and their variances †
Substituted hydrocarbons VCM plant Acrylonitrile plant	PENG-ROB, RK-SOAVE
Ether production MTBE, ETBE, TAME	WILSON, NRTL, UNIQUAC and their variances †
Ethylbenzene and styrene plants	PENG-ROB, RK-SOAVE –or– WILSON, NRTL, UNIQUAC and their variances †
Terephthalic acid	WILSON, NRTL, UNIQUAC and their variances † (with dimerization in acetic acid section)

† *See the figures on pages 7-10 through 7-12 for recommendations based on pressure and vapor phase association.*

Chemicals

Application	Recommended Property Methods
Azeotropic separations Alcohol separation	WILSON, NRTL, UNIQUAC and their variances†
Carboxylic acids Acetic acid plant	WILS-HOC, NRTL-HOC, UNIQ-HOC
Phenol plant	WILSON, NRTL, UNIQUAC and their variances†
Liquid phase reactions Esterification	WILSON, NRTL, UNIQUAC and their variances†

Continued

Application	Recommended Property Methods
Ammonia plant	PENG-ROB, RK-SOAVE
Fluorochemicals	WILS-HF
Inorganic Chemicals Caustic Acids Phosphoric acid Sulphuric acid Nitric acid Hydrochloric acid	ELECNRTL
Hydrofluoric acid	ENRTL-HF

† *See the figures on pages 7-10 through 7-12 for recommendations based on pressure and vapor phase association*

Coal Processing

Application	Recommended Property Methods
Size reduction crushing, grinding	SOLIDS
Separation and cleaning sieving, cyclones, precipitation, washing	SOLIDS
Combustion	PR-BM, RKS-BM (combustion databank)
Acid gas absorption with Methanol (RECTISOL) NMP (PURISOL)	PRWS, RKSWS, PRMHV2, RKSMHV2, PSRK, SR-POLAR
Acid gas absorption with Water Ammonia Amines Amines + methanol (AMISOL) Caustic Lime Hot carbonate	ELECNRTL
Coal gasification and liquefaction	See Synthetic Fuels table.

Power Generation

Application	Recommended Property Methods
Combustion Coal Oil	PR-BM, RKS-BM (combustion databank)
Steam cycles Compressors Turbines	STEAMNBS, STEAM-TA
Acid gas absorption	See gas processing.

Synthetic Fuel

Application	Recommended Property Methods
Synthesis gas	PR-BM, RKS-BM
Coal gasification	PR-BM, RKS-BM
Coal liquefaction	PR-BM, RKS-BM, BWR-LS

Environmental

Application	Recommended Property Methods
Solvent recovery	WILSON, NRTL, UNIQUAC and their variances †
(Substituted) hydrocarbon stripping	WILSON, NRTL, UNIQUAC and their variances †
Acid gas stripping from Methanol (RECTISOL) NMP (PURISOL)	PRWS, RKSWS, PRMHV2, RKSMHV2, PSRK, SR-POLAR
Acid gas stripping from: Water Ammonia Amines Amines + methanol (AMISOL) Caustic Lime Hot carbonate	ELECNRTL
Acids Stripping Neutralization	ELECNRTL

† *See the figures on pages 7-10 through 7-12 for recommendations based on pressure and vapor phase association.*

Water and Steam

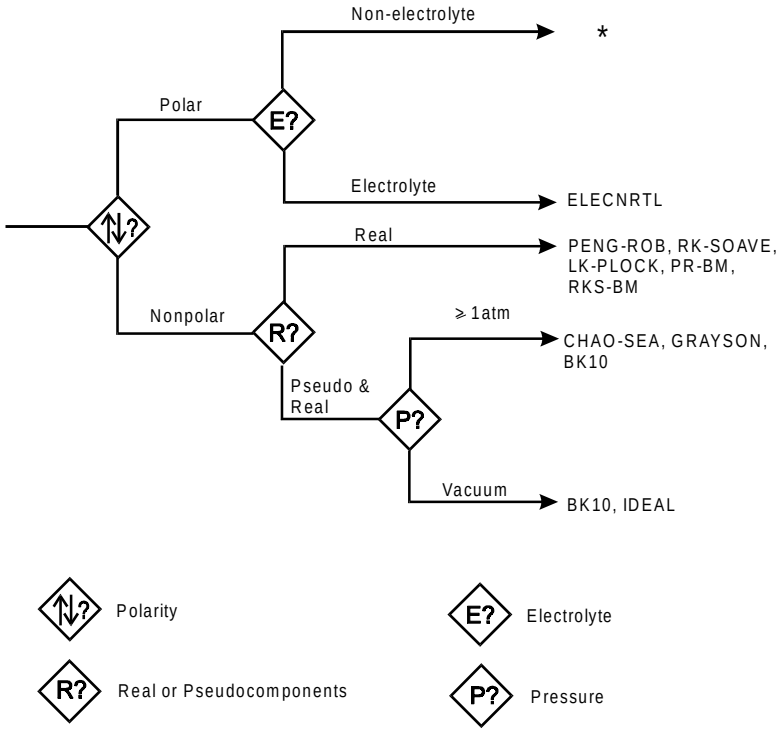
Application	Recommended Property Methods
Steam systems Coolant	STEAMNBS, STEAM–TA

Mineral and Metallurgical Processes

Application	Recommended Property Methods
Mechanical processing: Crushing Grinding Sieving Washing	SOLIDS
Hydrometallurgy Mineral leaching	ELECNRTL
Pyrometallurgy Smelter Converter	SOLIDS

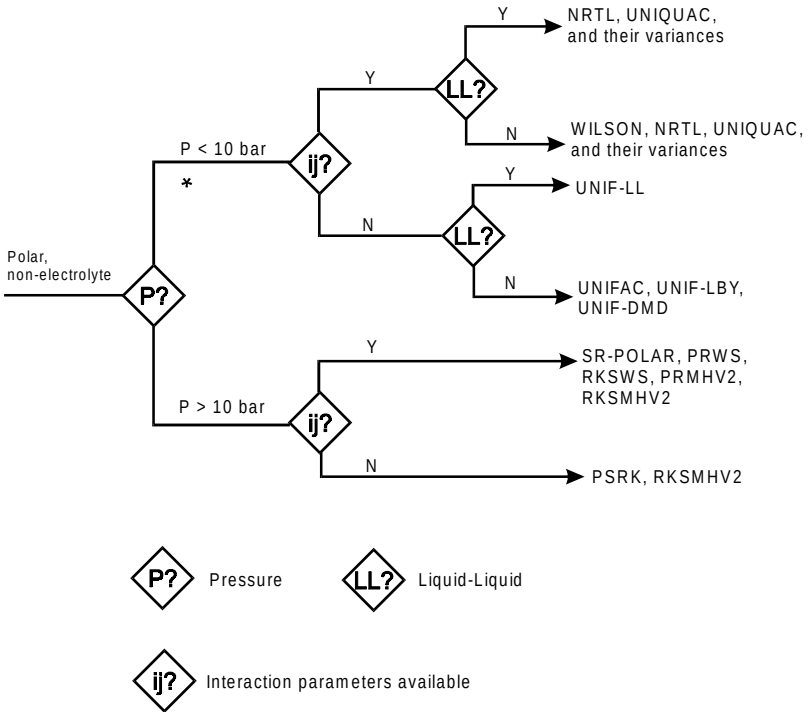
Guidelines for Choosing a Property Method

The following diagrams show the process for choosing a property method.



* See the figure on page 7-11.

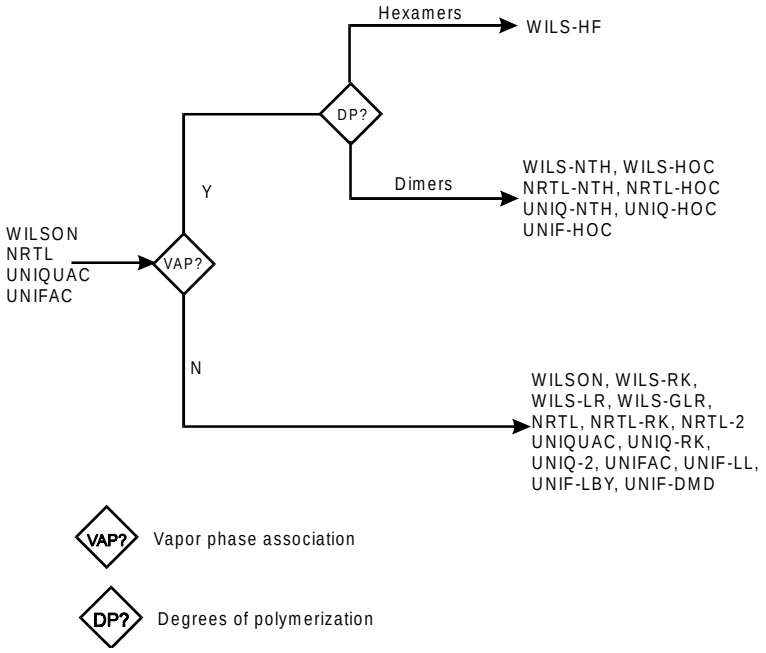
Guidelines for Choosing a Property Method



* See the figure on page 7-12 .

Guidelines for Choosing a Property Method for Polar Non-Electrolyte Systems

Guidelines for Choosing an Activity Coefficient Property Method



General Guidelines for Choosing an Activity Coefficient Property Method

Specifying the Global Property Method

Aspen Plus uses the global property method for all property calculations, unless you specify a different property method for a specific flowsheet section, unit operation block, or property analysis.

To specify the global property method:

1. From the Data menu, click Properties.
2. On the Global sheet, in the Property Method list box, specify the property method.
3. You can also use the Process Type list box to help you select an appropriate property method. In the Process Type list box, select the type of process you want to model. Each process type has a list of recommended property methods. For more information on process types, see Chapter 2.
4. In the Base Method list box, select a base property method.

5. If you are using an activity coefficient property method and want to use Henry's law for supercritical components, specify the Henry component list ID in the Henry Components list box. For more information on Henry's components, see Defining Supercritical Components on page 7-15.
6. If you have a petroleum application that requires free water calculations, specify the property method for the free water phase in the Free-Water Method list box and water solubility option in the Water Solubility list box. For more information, see Using Free Water Calculations on page 7-16.
7. For electrolyte applications, you must select an electrolytic property method, then select the Chemistry ID in the Chemistry ID list box. You can also specify the electrolyte computation method in the Use True-Components check box.

Specifying a Property Method for a Flowsheet Section

Use flowsheet sections to simplify the assignment of property methods when you are using more than one property method in a simulation. For example, you could divide a flowsheet into high pressure and low pressure sections, and assign an appropriate property method to each section.

See Chapter 3 for more information on flowsheet sections, including how to create a flowsheet section.

To specify a property method for a flowsheet section:

1. From the Data menu, click Properties
2. On the Flowsheet Sections sheet, select a flowsheet section from the Flowsheet Section ID list box.
3. Specify the property method in the Property Method list box.
4. You can also use the Process Type list box to help you select an appropriate property method. In the Process Type list box, select the type of process you want to model. Each process type has a list of recommended property methods. For more information on process types, see Chapter 2.
5. In the Base Method list box, select a base property method.
6. If you are using an activity coefficient property method and want to use Henry's Law for supercritical components, specify the Henry component list ID in the Henry Components list box. For more information on Henry's components, see Defining Supercritical Components on page 7-15.
7. For petroleum applications, you may want free water calculations. Specify the free water property method in the Free-Water Method list box and water solubility option in the Water Solubility list box. For more information, see Using Free Water Calculations on page 7-16.

8. For electrolyte applications, you must select an electrolytic property method, then select the Chemistry ID in the Chemistry ID list box. You can also specify the electrolyte computation method in the Use True-Components check box.

Specifying a Local Property Method

You can override the global property method by specifying a local property method on:

- The BlockOptions Properties sheet, for a unit operation block
- The Properties sheet, for a Properties Analysis

The specifications you enter on the Properties sheet apply only to that unit operation block or property analysis.

For the following unit operation models, you can specify different property methods for streams or sections in the block:

Model	Sheet	Allows you to specify property methods for
Decanter	Decanter Properties Phase Property	Liquid1 and liquid2 phases
RadFrac	Radfrac Properties Property Sections	Column segments, decanters, thermosyphon reboiler
RGibbs	Rgibbs Setup Products	Each phase
MultiFrac	Multifrac Properties Property Sections	Column segments
PetroFrac	Petrofrac Properties Property Sections Petrofrac Stripper Properties Property Sections	Column segments for main column Column segments for stripper
HeatX	Heatx BlockOptions Properties	Hot and cold sides of the exchanger
MHeatX	Mheatx BlockOptions Properties	Each stream in the exchanger
RPlug	Rplug BlockOptions Properties	Reactant and external coolant streams

Use the Properties Specifications Referenced sheet to enter additional property methods for use in the unit operation blocks or in property analysis calculations.

When performing an interactive property analysis, you can select any property method that has been specified on the Properties Specifications Referenced sheets.

Defining Supercritical Components

Activity coefficient property methods handle supercritical components present in the liquid phase by the asymmetric convention for activity coefficient normalization (Henry's law).

To use Henry's law for supercritical components:

1. Select an appropriate property method. These property methods allow Henry's law:

B-PITZER	NRTL-2	UNIQUAC	VANL-2
IDEAL	PITZER	UNIQ-HOC	WILSON
ELECNRTL	PITZ-HG	UNIQ-NTH	WILS-HF
ENRTL-HF	SOLIDS	UNIQ-RK	WILS-HOC
ENRTL-HG	UNIFAC	UNIQ-2	WILS-NTH
NRTL	UNIF-DMD	VANLAAR	WILS-RK
NRTL-HOC	UNIF-HOC	VANL-HOC	WILS-2
NRTL-NTH	UNIF-LBY	VANL-NTH	WILS-GLR
NRTL-RK	UNIF-LL	VANL-RK	WILS-LR

2. Define a Henry's component group using the Henry Comps forms. For more information, see Chapter 6.
3. Enter the ID of the Henry's component group on the Properties Specifications Global sheet (Use the Flowsheet Sections sheet for flowsheet sections specifications) or BlockOptions Properties sheet (local specification for unit operation models).

   For more information on Henry's law, see Aspen Plus *Physical Property Methods and Models.*

   Equation-of-state property methods do not require special treatment for supercritical components.

Using Free Water Calculations

For water-hydrocarbon applications, two liquid phases often coexist with a vapor phase. Aspen Plus has two approaches for modeling these types of vapor-liquid-liquid equilibrium simulations:

- Rigorous three-phase calculations
- Calculations with a free water approximation. When you use free water approximation, Aspen Plus assumes the water phase is pure liquid water (free water).

Free water calculations are:

- Normally adequate for water-hydrocarbon systems, where the hydrocarbon solubility in the water phase is generally negligible.
- Always faster than rigorous three-phase calculations, and require minimal physical property data.

For more information on requesting free water calculations, see Chapter 5.

Note You can also specify free water calculations on a local basis in individual streams and blocks. For more information on free-water calculations. see *Aspen Plus Physical Property Methods and Models*.

Specifying Properties for the Free Water Phase

When you use the free water approximation, you must specify the property method to be used for the free water phase. This property method calculates all thermodynamic and transport properties for the free-water phase.

To choose a property method:

1. Go to the Properties Specifications Global sheet or Flowsheet Sections sheet, or the BlockOptions Properties sheets for a unit operation model.
2. In the Free-Water Method list box, select one:

Property Method	Description	Merits
STEAM-TA	1967 ASME steam table correlations (default)	-
STEAMNBS	NBS/NRC steam table correlations	More accurate than the ASME steam table
IDEAL or SYSOP0	For systems at low or moderate pressures	More efficient calculations than STEAM-TA or STEAMNBS

Special Method for K-Value of Water in the Organic Phase

The global property method calculates the K-value of water unless you specify another method.

In free water calculations, you can use a special method to calculate the K-value of water in the organic phase:

$$K_w = \frac{\gamma_w \varphi_w^{*,l}}{\varphi_w^{v}}$$

Where:

γ_w	=	Activity coefficient of water in the organic phase
$\varphi_w^{*,l}$	=	Fugacity coefficient of pure liquid water calculated using the free-water phase property method
φ_w^{v}	=	Fugacity coefficient of water in the vapor phase mixture

To select a calculation method for γ_w and φ_w^{v}:

1. Go to the Properties Specifications Global or Flowsheet Sections sheet, or the BlockOptions Properties sheet for a unit operation model.
2. In the Water Solubility list box, select one:

Water Solubility Option	Calculates γ_w from††	Calculates φ_w^{v} from
0	$\gamma_w = \frac{1}{x_w^{sol}}$	Free-water property method
1	$\gamma_w = \frac{1}{x_w^{sol}}$	Primary property method
2	$\gamma_w = f(T, x_w)$ where $\gamma_w = \frac{1}{x_w^{sol}}$ when $x_w = x_w^{sol}$	Primary property method
3†	The K-value of water is calculated by the primary property method	

Note X_w^{sol} is solubility of water in the organic phase, calculated using the water-solubility correlation. (WATSOL).

† *Water solubility option 3 is not recommended unless binary interaction parameters regressed from liquid-liquid equilibrium data are available.*

†† X_w^{sol} *is solubility of water in the organic phase, calculated using the water-solubility correlation. (WATSOL).*

Specifying Electrolyte Calculations

To model an electrolyte system, you must:

- Use an electrolyte property method. ELECNRTL is recommended. Other property methods are PITZER, B-PITZER, ENRTL-HF, ENRTL-HG AND PITZ-HG.
- Define the solution chemistry on the Reactions Chemistry Stoichiometry sheet.
- Select the solution chemistry ID to be used with the electrolyte property method in the Chemistry ID list box on the Properties Specifications Global sheet or the Flowsheet Sections sheet or the BlockOptions Properties sheet of a unit operation model.
- Specify either the true or apparent component simulation approach using the Use True Components check box.

Use the button on the Components Specifications Selection sheet to open the Electrolytes Wizard which can set up all of these specifications for you. For information on how to use the Electrolyte Wizard, see Chapter 6.

Modifying Property Methods

Property methods are defined by calculation paths (routes) and physical property equations (models), which determine how properties are calculated.

Built-in property methods are sufficient for most applications. However, you can modify a property method to include, for example:

- A route that calculates liquid fugacity coefficients without the Poynting correction
- A route that calculates liquid enthalpy without heat of mixing
- A different equation-of-state model for all vapor phase property calculations
- A different set of parameters (for example, dataset 2) for an activity coefficient model
- A route that calculates liquid molar volume using the Rackett model, instead of a cubic equation of state

For more information on property models and model option codes, and on routes and how to create them, see *Aspen Plus Physical Property Methods and Models*.

Modifying a Built-in Property Method

You can make the above common modifications to a property method on the Properties Specifications Global sheet or the Flowsheet Section sheet:

1. From the Data menu, click Properties.
2. On the Global or the Flowsheet Sections sheet, select the property method you want to modify in the Base Method list box.
3. Check the Modify Property Models check box.
4. When prompted, enter a new name for your modified property method and click OK. Although it is not required, it is highly recommended that you specify a new name for the modified property method.

   You can make these modifications:

In this box	To do this
Vapor EOS	Select an equation of state model for all vapor phase properties calculations
Liquid gamma	Select an activity coefficient model
Data set	Specify parameter data set number for the EOS or liquid gamma model
Liquid enthalpy	Select a route to calculate liquid mixture enthalpy
Liquid volume	Select a route to calculate liquid mixture volume
Poynting correction	Specify whether or not the Poynting correction is used in calculating liquid frugacity coefficients. When selected, the Poynting correction is included.
Heat of mixing	Specify whether or not heat of mixing is included in liquid mixture enthalpy. When selected, heat of mixing is included.

Making Advanced Modifications to a Property Method

For additional and advanced modifications, use the Properties Property Methods form:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser, double-click the Property Methods folder.

   The Object Manager appears.
3. Select the Property Method you want to modify and click Edit.

   – or –

   To create a new property method, click New, then specify the new property method.

4. Use the Routes sheet to specify property routes and the Models sheet to specify property models.

The Routes sheet displays the base property method, the properties and route ID used to calculate each property. For convenience, properties are categorized as follows:

- Pure thermodynamic
- Mixture thermodynamic
- Pure transport
- Mixture transport

To modify a route in the property method, select a desired route in the Route ID box. You can also:

Click this button	To do this
Create	Create a new route for the selected property
Edit	Modify a selected route
View	View the structure of a selected route. The structure shows exactly how the route is calculated and by what methods and models.

The Models sheet displays the property models used for calculation of the properties in the property method. To modify a property model, select the desired model in the Model Name column.

This table describes the different boxes on the Models sheet:

Use this box	To specify
Model name	The model you want to use to calculate each property
Data set	The data set number for the parameters for the model

For a given model:

Use this button	To Get
Affected properties	A list of properties affected by the model. Models such as equation of state are used to calculate more than one property.
Option codes	Model option codes. Option codes are used to specify special calculation options.

Property Methods for Nonconventional Components

The only properties calculated for nonconventional components are enthalpy and density. The folllowing tables list the models available. See Aspen Plus Physical Property Methods and Models, Chapter 3, for detailed descriptions of these models.

Nonconventional Property Models

This table shows the general models:

Property	Model	Attribute Requirements
ENTHALPY	ENTHGEN	GENANAL
DENSITY	DNSTYGEN	GENANAL

This table shows the special models for coal and coal-derived materials:

Property	Model	Attribute Requirements
ENTHALPY	HCOALGEN	ULTANAL, PROXANAL, SULFANAL
	HCJ1BOIE	ULTANAL, PROXANAL, SULFANAL
	HCOAL-R8	ULTANAL, PROXANAL, SULFANAL
	HBOIE-R8	ULTANAL, PROXANAL, SULFANAL
DENSITY	DCOALIGT	ULTANAL, SULFANAL
	DCHARIGT	ULTANAL, SULFANAL

The tabular models for nonconventional components are:

Property	Model
ENTHALPY	ENTHLTAB
DENSITY	DNSTYTAB

Specifying the Models for Nonconventional Components

To specify the models used to calculate physical properties for nonconventional components:

1. From the Data menu, click Properties.

2. Double-click the Advanced folder.
3. Select the NC-Props form.
4. Select a component in the Component list box of the Property Methods sheet.
5. Specify the models for enthalpy and density.

   Aspen Plus automatically fills in the required component attributes for the models you specified.

8 Physical Property Parameters and Data

This chapter explains how to evaluate property parameter requirements, determine parameters available from databanks, and enter additional parameters and data.

Topics include:

- About parameters and data
- Determining property parameter requirements
- Retrieving parameters from databanks
- Entering property parameters
- Using tabular data and polynomial coefficients
- Using property data packages

About Parameters and Data

When beginning any new simulation, it is important to check that you have correctly represented the physical properties of your system. After you select the property methods for a simulation as described in the previous chapter, you must determine property parameter requirements and ensure that all required parameters are available.

In order to understand this and subsequent chapters, it is important to distinguish between the terms Parameters and Data:

Item	Definition	Example
Parameters	The constants used in the many different physical property models, or equations, used by Aspen Plus to predict physical properties	These can be scalar constants such as molecular weight (MW) and critical temperature (TC), or they can be temperature-dependent property correlation parameters such as the coefficients for the extended Antoine vapor pressure equation (PLXANT).
Data	Raw experimental property data that can be used for estimation or regression of parameters	Vapor pressure vs. Temperature data could be used to estimate or regress the extended Antoine parameters (PLXANT).

Determining Property Parameter Requirements

Depending on the type of simulation, your model will require different parameters. The following sections describe the parameter requirements for some basic property calculations, that is, for:

- Mass and energy balance simulations
- Henry's law
- Thermodynamic reference state

Most equation-of-state and activity coefficient models require binary parameters for meaningful results. To determine parameter requirements based on your chosen property methods, see the Property Method Tables in Aspen Plus Physical Property Methods and Models for each property method you select.

Parameter Requirements for Mass and Energy Balance Simulations

For simulations that involve both mass and energy balance calculations, you must enter or retrieve from the databanks these required parameters:

Enter or retrieve this parameter	For	On this type of Properties Parameters form
MW	Molecular weight	Pure Component Scalar
PLXANT	Extended Antoine vapor pressure model	Pure Component T-Dependent
CPIG or CPIGDP	Ideal gas heat capacity model	Pure Component T-Dependent
DHVLWT or DHVLDP	Heat of vaporization model	Pure Component T-Dependent

This table gives further information:

If you	These parameters are required	Enter them on this type of Properties Parameters form
Use the standard liquid volume basis for any flowsheet or unit operation model specification	Standard liquid volume parameters (VLSTD)	Pure Component Scalar
Request free-water calculations	Parameters for the water solubility model (WATSOL)	Pure Component T-Dependent

Tip If you deselect the Perform Heat Balance Calculations option on the Setup Simulation Options Calculations sheet, Aspen Plus does not calculate enthalpies, entropies, or Gibbs free energies. It does not require the parameters used to compute these properties.

Parameter Requirements for Henry's Law

If you use Henry's law for supercritical components (or dissolved-gas components), Henry's constant model parameters (HENRY) are required for all dissolved-gas components with the solvents. You must list the supercritical components on the Components Henry Comps Selection sheet.

If	You require these parameters
More than one solvent is in the mixture	Henry's constant parameters for each dissolved-gas solvent pair.
Henry's constants are not available for all solvents	Henry's constants for the major solvents. Aspen Plus uses a rigorous defaulting procedure when Henry's constants are missing for a minor solvent component.

Enter Henry's constant model parameters on the Input sheet of the HENRY-1 object on the Properties Parameters Binary Interaction HENRY-1 form.

Parameter Requirements for Thermodynamic Reference State

The reference state for thermodynamic properties is the constituent elements in an ideal gas state at 25° C and 1 atm. To calculate enthalpies, entropies, and Gibbs free energies, Aspen Plus uses:

- Standard heat of formation (DHFORM)
- Standard Gibbs free energy of formation (DGFORM)

For systems that do not involve chemical reaction, you may allow DHFORM and DGFORM to default to zero.

Values of	Must be available for all components
DHFORM	Participating in chemical reactions
DGFORM	Involved in equilibrium reactions modeled by the RGibbs reactor model

Reference State for Conventional Solid Components

Conventional solid components may require:

- Standard solid heat of formation (DHSFRM)
- Standard solid Gibbs free energy of formation (DGSFRM)

Enter them on the Properties Parameters Pure Component Scalar Input sheet.

Reference State for Ionic Species

The reference state for ionic species is infinite dilution in water. To calculate enthalpy, entropy, and Gibbs free energy of ions, Aspen Plus uses:

- Standard heat of formation in water at infinite dilution (DHAQFM)
- Standard Gibbs free energy of formation in water at infinite dilution (DGAQFM)

Retrieving Parameters from Databanks

For many components, Aspen Plus databanks store all required parameter values. This chapter explains how to retrieve these built-in parameters from Aspen Plus databanks:

- Pure component parameters
- Equation-of-state binary parameters
- Activity coefficient binary parameters
- Henry's Law constants
- Electrolyte and binary pair parameters

Retrieving Pure Component Parameters

For many components, Aspen Plus retrieves pure component parameters automatically from its pure component databanks. Use the Components Specifications Databanks sheet to specify the databanks to search and their search order. Parameters missing from the first selected databank will be searched for in subsequent selected databanks.

To enter your own parameter values, use the Properties Parameters Pure Component Scalar Input and T-Dependent Input sheets. See Entering Pure Component Constants on page 8-11.

Since built-in pure component databanks reside with the simulation engine, the available parameters do not appear automatically on any Parameters Pure Component Input sheets.

User entered parameters override values retrieved from the Aspen Plus databanks.

To generate a report of all available pure component parameters that will be used in the simulation for the components and property methods specified:

1. From the Tools menu, click Retrieve Parameters Results.
2. On the Retrieve Parameter Results dialog box, click OK to generate a report.
3. On the next Retrieve Parameter Results dialog box, click OK to view the results.

   The Data Browser automatically opens at the Properties Parameters Results folder.
4. In the left pane of the Data Browser, choose the Pure Component form from the Results folder.

The Parameters Results Pure Components form contains a sheet for scalar parameters and a sheet for T-Dependent parameters. On each sheet you can choose to view the actual parameter values, or the status. For the status of parameter results, the following status is possible:

Status	Indicates the parameter is
Available	Available in the databank, entered on the Paramters Input sheet, estimated, or regressed
Default	A system default value
Missing	Missing

In addition to retrieving parameter results with the method described above, you can also generate a detailed parameter report in the Aspen Plus report file. For details on this and other report options see Chapter 12.

Retrieving Equation-of-State Binary Parameters

For many component systems, binary parameters are available for these models:

Model	Parameter name
Standard Redlich-Kwong-Soave	RKSKIJ
Standard Peng-Robinson	PRKIJ
Lee-Kesler-Plöcker	LKPKIJ
BWR-Lee-Starling	BWRKV, BWRKT
Hayden-O'Connell	HOCETA

Aspen Plus retrieves any databank values and uses them automatically. Whether you enter these parameters yourself or retrieve them from a databank, you can view them from the appropriate Properties Parameters Binary Interaction Input sheet. Aspen Plus creates one form for each binary parameter.

If you do not want to retrieve built-in equation-of-state binary parameters, remove the databank name from the Selected Databanks list on the Databanks sheet of the Properties Parameters Binary Interaction form for your equation-of-state model. Use the Input sheet to enter your own binary parameter values. For more information see Entering Scalar Binary Parameters on page 8-16.

Retrieving Activity Coefficient Binary Parameters

For many component pairs, binary parameters are available for the following property methods for vapor-liquid applications:

Property method	Parameter name
NRTL	NRTL
NRTL-HOC	NRTL
NRTL-RK	NRTL
UNIQUAC	UNIQ
UNIQ-HOC	UNIQ
UNIQ-RK	UNIQ
WILSON	WILSON
WILS-HOC	WILSON
WILS-GLR	WILSON
WILS-LR	WILSON
WILS-RK	WILSON

For liquid-liquid applications, binary parameters are available for the following property methods:

Property method	Parameter name
NRTL	NRTL
NRTL-HOC	NRTL
NRTL-RK	NRTL
UNIQUAC	UNIQ
UNIQ-HOC	UNIQ
UNIQ-RK	UNIQ

AspenTech developed these parameters using data from the Dortmund Databank. See *Aspen Plus Physical Property Data* for details.

Whenever you select these property methods, Aspen Plus retrieves these parameters automatically and displays them on the Input sheet of the Properties Parameters Binary Interaction forms. Aspen Plus creates a form for each binary parameter.

If you do not want to retrieve built-in binary parameters, remove the databank name from the Selected Databanks list on the Databanks sheet of the Properties Parameters Binary Interaction form. Use the Input sheet to enter your own binary parameter values.

For more information, see Entering Temperature-Dependent Binary Parameters on page 8-17.

For binary parameters retrieved from a databank, use Help to obtain information about the quality of the parameters—for example, sum of squares error and average and maximum deviations of the fit.

Retrieving Henry's Law Constants

Henry's law constants are available for a large number of solutes in solvents. The solvents are water and many organic components.

If you use an activity coefficient property method and define a set of Henry's components, Aspen Plus retrieves the Henry's constants automatically and displays them on the Input sheet of the Properties Parameters Binary Interaction HENRY-1 form.

If you do not want to retrieve built-in Henry's law constants, remove both the BINARY and HENRY databanks from the Selected Databanks list on the Databanks sheet of the HENRY-1 form.

Retrieving Electrolyte Binary and Pair Parameters

Binary and pair parameters of the Electrolyte NRTL model are available for many industrially important electrolyte systems.

Aspen Plus retrieves the binary parameters and displays them on the Properties Parameters Binary Interaction forms. For pair parameters, Aspen Plus displays them on the Properties Parameters Electrolyte Pair forms.

If you do not want to retrieve built-in parameters, remove the databank name from the Selected Databanks list on the Databanks sheet of the applicable form.

See *Aspen Plus Physical Property Data*, Chapter 2, for details about electrolyte systems, the sources of data used, and the application range.

Entering Property Parameters

If any parameters required by your simulation are missing from the databanks, or if you do not want to use databank values, you can:

- Enter any parameters or data directly.
- Estimate parameters using Property Estimation. For more information, see Chapter 30.
- Regress parameters from experimental data using Data Regression. For more information, see Chapter 31.

This section explains how to enter the following parameters directly:

-
- Pure component constants
- Pure component correlation parameters
- Parameters for nonconventional components
- Scalar binary parameters
- Temperature-dependent binary parameters
- Binary parameters from Dechema
- Electrolyte pair parameters
- Ternary parameters

Forms for Entering Property Parameters

The table below shows where to enter the different types of property parameters:

Use the Input sheet of this Properties Parameters form	To enter
Pure Component Scalar	Scalar pure component parameters, such as critical temperature (TC) or molecular weight (MW)
Pure Component T-Dependent	Temperature-dependent pure component property correlation parameters, such as PLXANT for the extended Antoine vapor pressure model
Pure Component Nonconventional	Unary parameters for nonconventional components
Binary Interaction	Scalar binary parameters, such as the RKSKIJ binary parameters for the Redlich-Kwong-Soave equation-of-state model Temperature-dependent binary parameters (that is, parameters defined with more than one element) such as the NRTL binary parameters or Henry's law constants
Electrolyte Pair	Electrolyte-molecule and electrolyte-electrolyte pair parameters required by the electrolyte NRTL model, such as the GMELCC parameters

Continued

Use the Input sheet of this Properties Parameters form	To enter
Electrolyte Ternary	Electrolyte ternary parameters required by the Pitzer model, such as the cation1-cation2-common anion parameters and anion1-anion2-common cation parameters (GMPTPS)
UNIFAC Group	Area and volume parameters for the UNIFAC functional groups
UNIFAC Group Binary	Scalar group-group interaction parameters for the original UNIFAC model (GMUFB) T-Dependent group-group interaction parameters for the modified UNIFAC models, such as the Dortmund-modified UNIFAC and the Lyngby-modified UNIFAC models

How to Enter Property Parameters

The general procedure for entering all property parameters is as follows. For details on entering the specific types of parameter, see the appropriate sections later in this chapter.

To enter property parameters:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser, double-click the Parameters folder.
3. Click the folder for the type of parameters you want to enter (Pure Component, Binary Interaction, Electrolyte Pair, Electrolyte Ternary, UNIFAC Group, or UNIFAC Group Binary). Descriptions for these parameter types are in the above table.

   Aspen Plus automatically creates parameter sets for any binary interaction, electrolyte pair, and parameters required by the property methods specified on the Properties Specifications form. The Object Manager for the appropriate parameter type displays the IDs for these parameter sets.
4. On the Object Manager for the parameter type you choose, you can
   - Enter parameters for an existing parameter set by selecting the parameter and clicking Edit.

     – or –
   - Create a new parameter set. In the Object Manager, click New. If prompted, select the appropriate parameter type and parameter name, and click OK.
5. Use the Parameter input sheet to:
   - Enter parameters that are not in the Aspen Plus databanks

- Override defaults or databank values by entering parameter values

You can enter parameter values in any units. After you specify a parameter name, Aspen Plus automatically fills in the default units.

If you change the units of measurement for the parameter after you enter the parameter value, Aspen Plus does not convert the displayed value.

Tip When defining non-databank components using the Components Specifications Selection sheet, you can use the User Defined Components Wizard. The wizard guides you through entering the basic pure component parameters required.

For more detailed information on the User Defined Components Wizard, see Chapter 6.

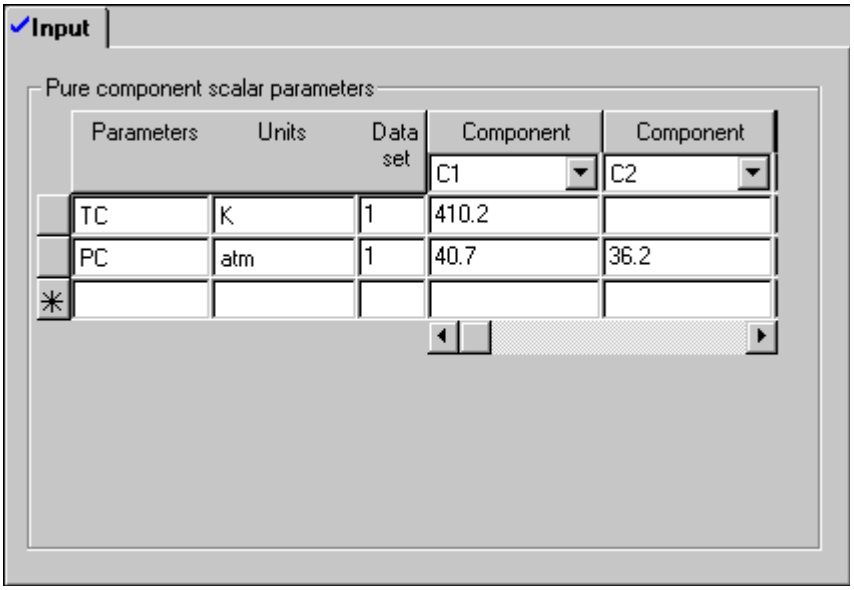
Entering Pure Component Constants

To enter pure component constants:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser, double-click the Parameters folder.
3. Click the Pure Component folder.
4. In the Parameters Pure Component Object Manager, you can create new parameter IDs, or modify existing IDs.
5. To create a new parameter set, on the Object Manager click New.
6. In the New Pure Component Parameters dialog box, the default parameter type is Scalar. Enter an ID or accept the default ID and click OK.
7. To modify an existing parameter ID, on the Object Manager select the name of the parameter set, and click Edit.
8. On the Input sheet for pure component scalar parameters, define the matrix of components and parameters for which you are entering data values, and specify the appropriate units.

Example of Entering Pure Component Constants

Enter critical temperature (TC) and critical pressure (PC) of 410.2 K and 40.7 atm for component C1. Enter critical pressure of 36.2 atm for component C2.

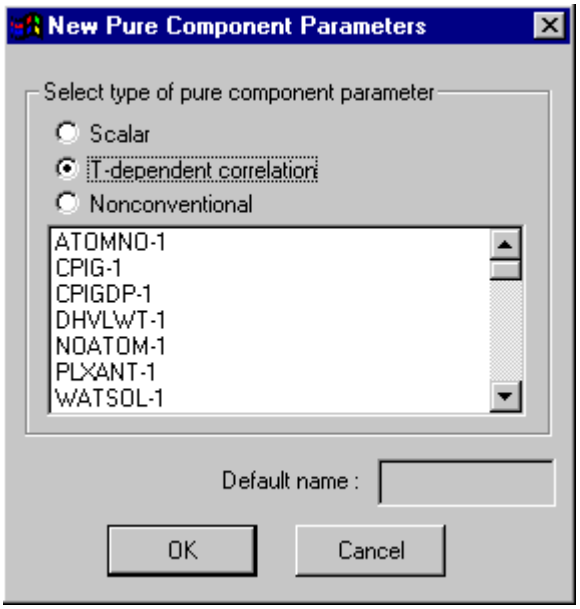


Entering Pure Component Correlation Parameters

To enter coefficients for temperature-dependent pure component property correlations:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser, double-click the Parameters folder.
3. Click the Pure Component folder.
4. In the Parameters Pure Component Object Manager, you can create new parameter IDs, or modify existing IDs.
5. To create a new parameter set, on the Object Manager click New.

The New Pure Component Parameters dialog box appears:



6. In the New Pure Component Parameters dialog box, select T-dependent correlation, and choose the appropriate parameter name from the list.
7. Click OK.
8. To modify an existing parameter ID, on the Object Manager select the name of the parameter set, and click Edit.
9. On the Input sheet, choose a component from the Component list. For the chosen temperature dependent parameter, use this sheet to enter values for all components for which you have parameters.
10. Specify the appropriate units and enter the coefficients of each parameter as sequential elements. For a more detailed description of models and parameters, see *Aspen Plus Physical Property Methods and Models*.

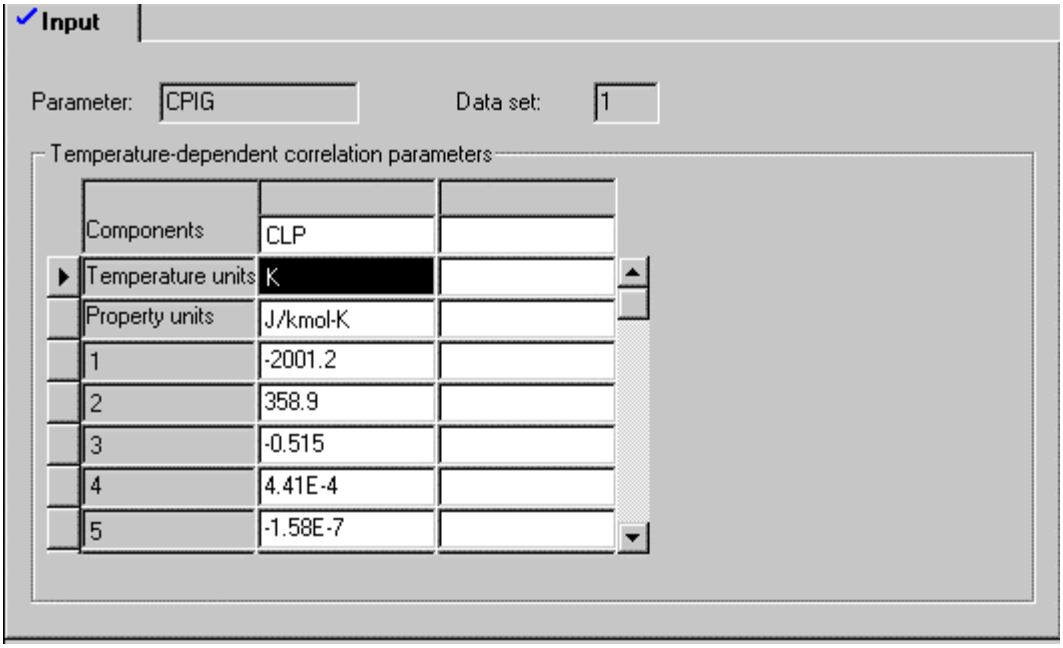
    You cannot enter more than one set of values for the same parameter on the same form.

Example for Entering Ideal Gas Heat Capacity Coefficients

For component CLP, enter the coefficients for the Ideal Gas Heat Capacity Polynomial model (CPIG):

$$C_P^{IG} = -2001.2 + 358.9T - 0.515T^2 + 4.41 \times 10^{-4}T^3 - 1.58 \times 10^{-7}\ T^4$$

C_P^{IG} has units of J/kmol-K. T is in units of K.

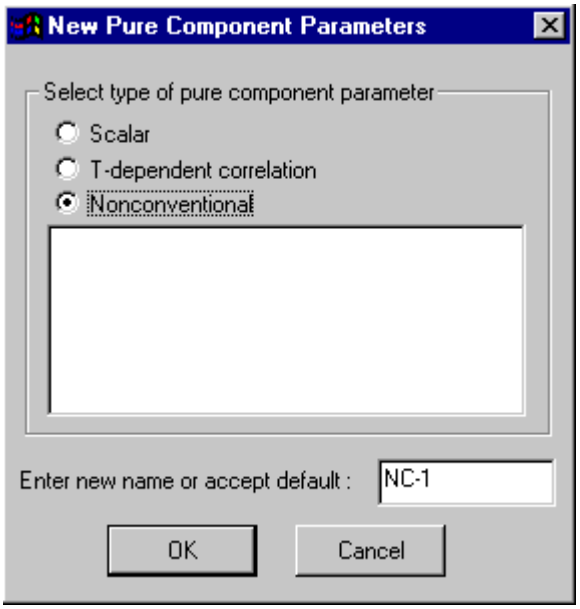


Entering Parameters for Nonconventional Components

To enter parameter values for nonconventional components:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser, double-click the Parameters folder.
3. Click the Pure Component folder.
4. In the Parameters Pure Component Object Manager, you can create new parameter IDs, or modify existing IDs.
5. To create a new parameter set, on the Object Manager click New.

The New Pure Component Parameters dialog box appears:



6. In the New Pure Component Parameters dialog box, select Nonconventional.
7. Enter an ID or accept the default ID, then click OK.
8. To modify an existing parameter ID, on the Object Manager select the name of the parameter set, and click Edit.
9. On the Input sheet, choose a parameter from the Parameter list.
10. Enter components, parameters, and units.

When you use the general enthalpy and density models shown in this table Aspen Plus requires at least the first element of the heat capacity polynomial (HCGEN) and density polynomial (DENGEN), for each constituent of each nonconventional component. The heat of formation (DHFGEN) is required when reactions occur involving nonconventional components:

General Models

Property	Model	Attribute Requirements
ENTHALPY	ENTHGEN	GENANAL
DENSITY	DNSTYGEN	GENANAL

Special Models for Coal and Coal-Derived Materials

Property	Model	Attribute Requirements
ENTHALPY	HCOALGEN	ULTANAL, PROXANAL, SULFANAL
	HCJ1BOIE	ULTANAL, PROXANAL, SULFANAL
	HCOAL-R8	ULTANAL, PROXANAL, SULFANAL
	HBOIE-R8	ULTANAL, PROXANAL, SULFANAL
DENSITY	DCOALIGT	ULTANAL, SULFANAL
	DCHARIGT	ULTANAL, SULFANAL

Alternatively, you can enter tabular data directly for enthalpy and density. Polynomial TABPOLY models are not available for nonconventional components.

Property	Model
ENTHALPY	ENTHLTAB
DENSITY	DNSTYTAB

For more information on using tabular data and polynomial coefficients see Using Tabular Data and Polynomial Coefficients on page 8-24.

Entering Scalar Binary Parameters

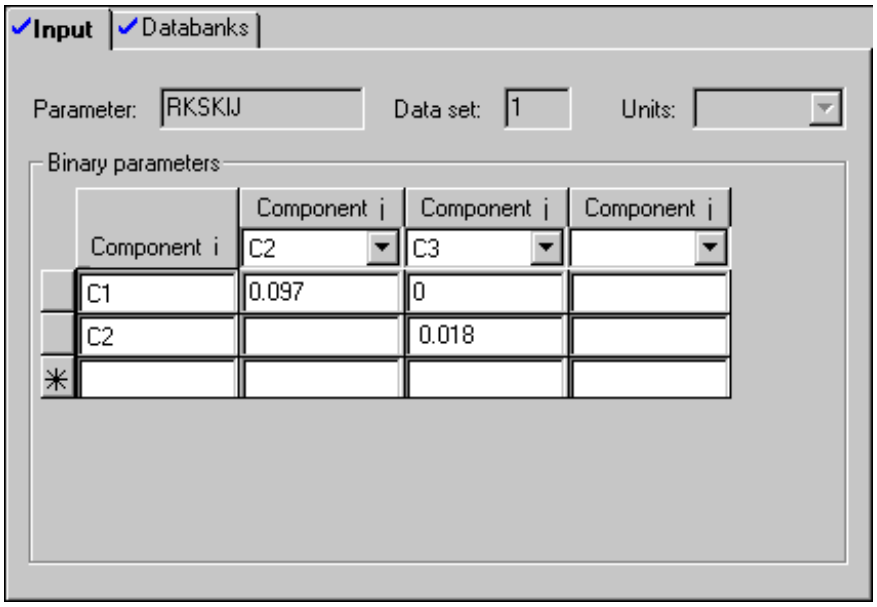
To enter scalar binary parameters:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser, double-click the Parameters folder.
3. Click the Binary Interaction folder to open the Object Manager containing the binary parameter sets used by your specified property methods.
4. On the Object Manager, select the scalar parameter of interest and click Edit.
5. Define the ij matrix of components for which you are entering binary parameter values.
6. Enter the parameter values.

Example for Entering Redlich-Kwong-Soave Binary Parameters

Binary parameters for the Redlich-Kwong-Soave equation of state, RKSKIJ, are symmetric (that is, $k_{ij} = k_{ji}$). Enter the following values for the binary parameters in the three-component system C1-C2-C3:

Component Pair	RKSKIJ
C1-C2	0.097
C1-C3	0
C2-C3	-0.018



Note You will not see the RKSKIJ-1 parameter in the Binary Interaction Object Manager unless you have previously chosen the RK-SOAVE property method. (See Chapter 7 for specifying property methods.)

Entering Temperature-Dependent Binary Parameters

To enter temperature-dependent binary parameters:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser, double-click the Parameters folder.
3. Click the Binary Interaction folder to open the Object Manager containing the binary parameter sets used by your specified property methods.

4. On the Object Manager, select the temperature-dependent parameter of interest (for example, NRTL-1) and click Edit.
5. On the Input sheet, enter component pairs in the Component i and Component j boxes.
6. Specify the units for the binary parameters.
7. Enter the coefficients of the parameters as sequential elements for each component pair.

Example for Entering NRTL Binary Parameters

The NRTL binary parameters a_{ij} and b_{ij} are asymmetric, that is, $a_{ij} \neq a_{ji}$ and $b_{ij} \neq b_{ji}$. The binary parameter c_{ij} and d_{ij} are symmetric; e_{ij} and f_{ij} default to zero. Enter the following NRTL binary parameters for the components C1-C2. The units for the binary parameters are in Kelvins.

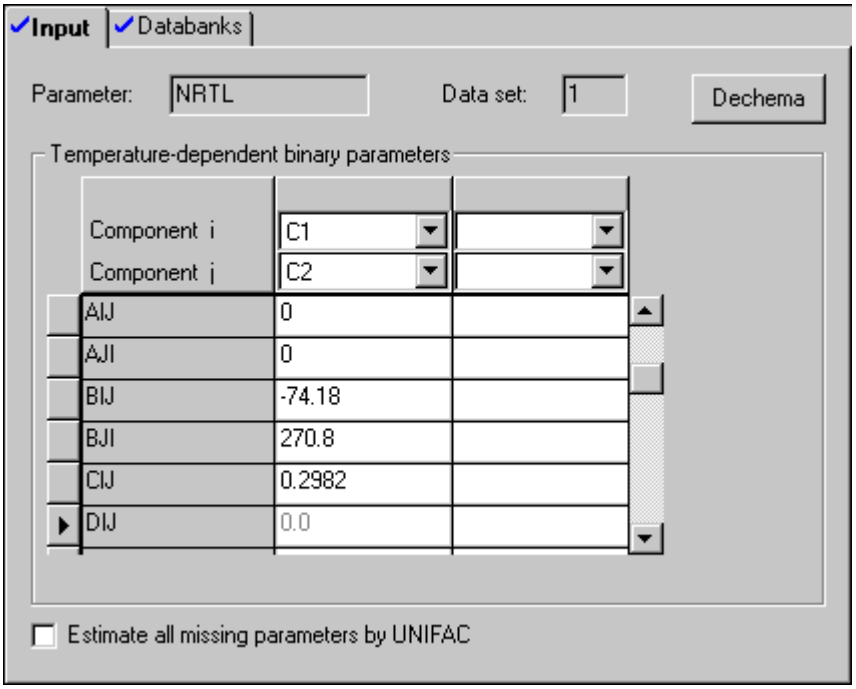
$a_{12} = 0$

$a_{21} = 0$

$b_{12} = -74.18$

$b_{21} = 270.8$

$c_{12} = 0.2982$



Note You will not see the NRTL-1 parameters in the Binary Interaction Object Manager, unless you have previously chosen an NRTL-based property method. (For information on specifying property methods, see Chapter 7.)

Entering Binary Parameters from DECHEMA

The DECHEMA Chemistry Data Series contains a large number of binary parameters for the Wilson, NRTL, and UNIQUAC models. These binary parameters are not compatible with the form of the equations used in Aspen Plus. However, you can enter them directly, without any conversion, using the Dechema button on the Properties Parameters Binary Interaction Input sheet for temperature dependent parameters.

To enter binary parameters from DECHEMA:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser, double-click the Parameters folder.
3. Click the Binary Interaction folder to open the Object Manager containing the binary parameter sets used by your specified property methods.
4. On the Object Manager, select NRTL-1, WILSON-1, or UNIQ-1 and choose Edit.
5. On the Input sheet, enter component pairs in the Component i and Component j boxes.
6. With the appropriate component pair selected, click the Dechema button.
7. In the Dechema Binary Parameters dialog box, enter the binary parameter values. You can also specify whether the parameters came from the VLE or LLE collection.
8. Click OK.

   Aspen Plus converts the binary parameters you enter and displays the converted values on the Input sheet.

   Aspen Plus databanks contain both parameters developed by Aspen Technology, Inc. and those obtained from the DECHEMA Chemistry Data Series (databank name = VLE-LIT). You will seldom need to enter binary parameters from the DECHEMA Chemistry Data Series.

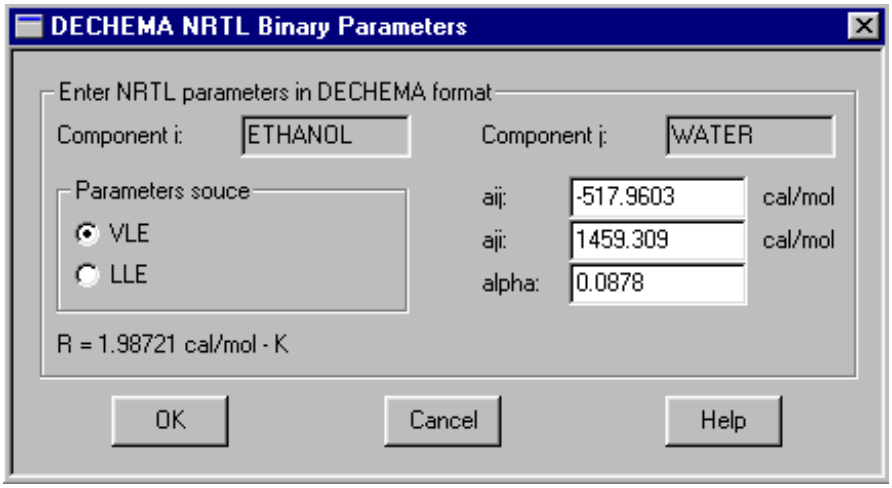
Example of Entering NRTL Binary Parameters from DECHEMA

Enter the following binary parameters for ethanol (i) and water (j), as reported in the DECHEMA Chemistry Data Series, Vol. I, Part 1A, p. 129:

a_{ij} = -517.9603 cal/mol

a_{ji} = 1459.309 cal/mol

α_{ij} = 0.0878



Estimating Binary Parameters for Activity Coefficient Models

You can request the estimation of missing binary parameters for the Wilson, NRTL, and UNIQUAC models, using the Properties Parameters Binary Interaction form. For convenience, Aspen Plus provides this capability in addition to the Property Constant Estimation System (PCES). For more information about PCES, see Chapter 30.

To estimate binary parameters:

1. Go to the Properties Parameters Binary Interaction Object Manager.
2. Select the WILSON-1, NRTL-1 or UNIQ-1 binary parameter form of interest and choose Edit.
3. On the Input sheet, check the Estimate All Missing Parameters by UNIFAC check box.

Entering Electrolyte Pair Parameters

Use the Properties Parameters Electrolyte Pair form to enter values for molecule-electrolyte and electrolyte-electrolyte pair parameters for the Electrolyte NRTL model.

To enter electrolyte pair parameters:

1. From the Data menu, click Properties.

2. In the left pane of the Data Browser, double-click the Parameters folder.
3. Click the Electrolyte Pair folder.
4. On the Electrolyte Pair Object Manager, select a parameter name, and click Edit.
5. On the Input sheet, define the molecule-electrolyte or electrolyte-electrolyte pairs for which you are entering values.
6. Enter the parameter values for the specified pairs.

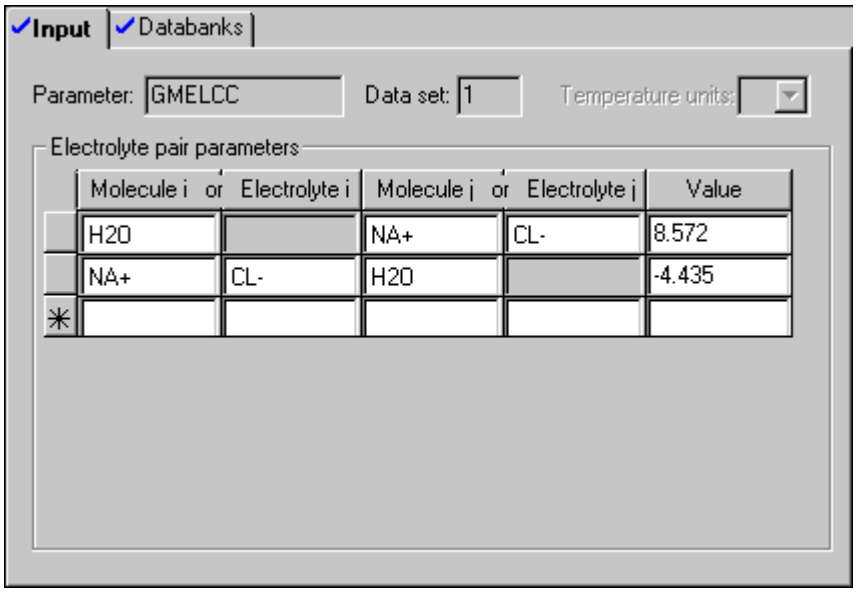
Example of Entering Electrolyte NRTL Pair Parameters

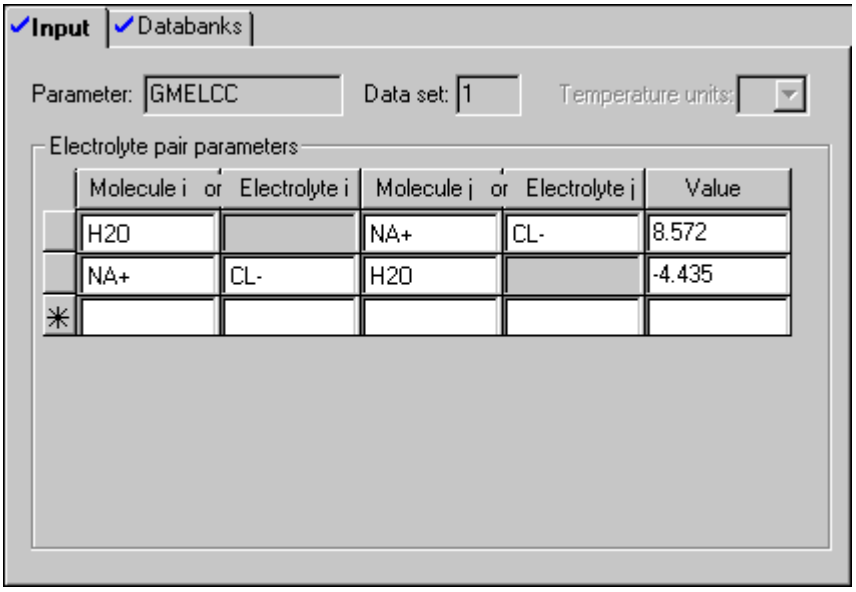
Enter the following electrolyte NRTL pair parameters (GMELCC) for the brine system:

$\tau_{H2O,NaCl}$ = 8.572

$\tau_{NaCl,H2O}$ = -4.435

NaCl dissociates completely into Na+ and Cl-.





Entering Ternary Parameters

Use the Properties Parameters Electrolyte Ternary form to enter values for the Pitzer ternary parameters when using the Pitzer electrolyte activity coefficient model.

For example, you can enter cation1-cation2-common anion parameters and anion1-anion2-common cation parameters (GMPTPS).

To enter electrolyte pair parameters:

1. From the Data menu, click Properties.
1. In the left pane of the Data Browser, double-click the Parameters folder.
2. Click the Electrolyte Ternary folder.
3. In the Electrolyte Ternary Object Manager, you can create new parameter IDs, or modify existing IDs.
4. To create a new parameter set, on the Object Manager click New.
5. In the Create New ID dialog box, enter an ID in the Enter ID box, or accept the default ID.
6. Click OK.
7. To modify an existing parameter ID, on the Object Manager select the name of the parameter set, and click Edit.
8. Select an electrolyte ternary parameter from the Parameter list.

9. With Cation selected in the View list, enter the cation1-cation2-common anion parameters by listing two cations, the common aion(s), and the respective parameter values. Enter all cation1-cation2-common anion parameters with the Cation view selected.
10. Select Anion from the View list.
11. Enter the anion1-anion2-common cation parameters by listing two anions, the common cation(s), and the respective parameter values. With the Anion view selected, continue to list all anion1-anion2-common cation parameters.

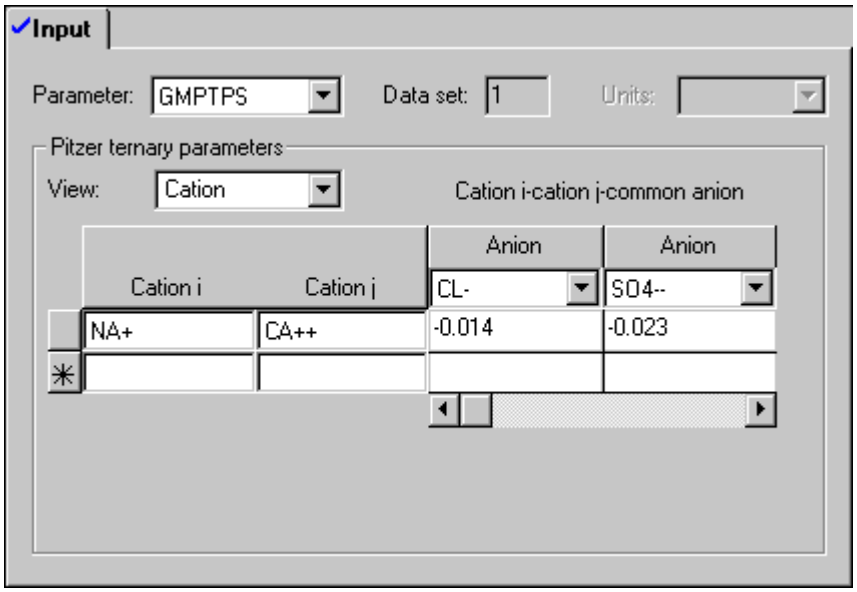
For more information on using the electrolyte features with Aspen Plus, see Chapter 6.

Example for Entering Electrolyte Pitzer Ternary Parameters

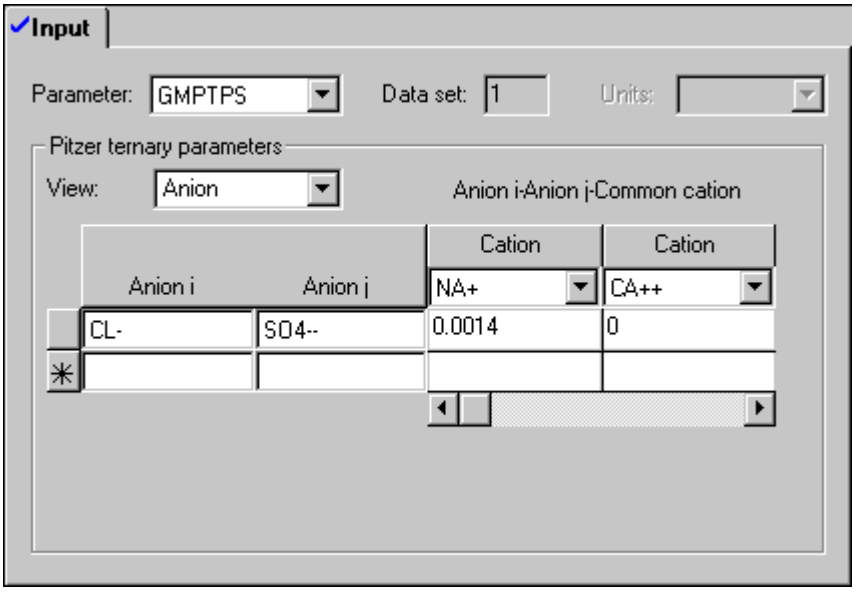
Enter the following Pitzer ternary parameters (GMPTPS) for the NaCl/CaSO4 system:

i	j	k	ψ_{ijk}
Na+	Ca+2	Cl-	-0.014
Na+	Ca+2	SO4-2	-0.023
Cl-	SO4-2	Na+	0 .0014
Cl-	SO4-2	Ca+2	0.0

Cation view:



Anion view:



Using Tabular Data and Polynomial Coefficients

In addition to the standard Aspen Plus physical property methods and models, you can represent some properties through:

- Direct use and interpolation of user-supplied tabular data
- Calculation from a general polynomial model

This section describes:

- Entering tabular data
- Entering polynomial coefficients for general polynomial model
- Adjusting reference states for tabular data and polynomials
- Adjusting tabular data or polynomials for the effect of pressure

This table shows the Tabpoly properties:

Property	Model Form†
Density for non-conventional components	Normal
Enthalpy for non-conventional components	Normal
Enthalpy of fusion	Normal

Continued

Property	Model Form
Enthalpy of sublimation	Normal
Enthalpy of vaporization	Normal
Henry's constant	Logarithmic
Ideal gas enthalpy	Normal
Ideal gas heat capacity	Normal
Liquid diffusion coefficient	Normal
Liquid enthalpy	Normal
Liquid enthalpy departure	Normal
Liquid entropy	Normal
Liquid entropy departure	Normal
Liquid fugacity coefficient for a component in a mixture	Logarithmic
Liquid Gibbs free energy	Normal
Liquid Gibbs free energy departure	Normal
Liquid heat capacity	Normal
Liquid-Liquid K-value	Logarithmic
Liquid thermal conductivity	Normal
Liquid viscosity	Logarithmic
Liquid volume	Normal
Pure component liquid fugacity coefficient	Logarithmic
Pure component vapor fugacity coefficient	Logarithmic
Solid enthalpy	Normal
Solid enthalpy departure	Normal
Solid entropy	Normal
Solid entropy departure	Normal
Solid fugacity coefficient	Logarithmic
Solid Gibbs free energy	Normal
Solid Gibbs free energy departure	Normal
Solid heat capacity	Normal
Solid thermal conductivity	Normal
Solid vapor pressure	Logarithmic
Solid volume	Normal
Surface tension	Normal
Vapor diffusion coefficient	Normal

Continued

Property	Model Form
Vapor enthalpy	Normal
Vapor enthalpy departure	Normal
Vapor entropy	Normal
Vapor entropy departure	Normal
Vapor fugacity coefficient for a component in a mixture	Logarithmic
Vapor Gibbs free energy	Normal
Vapor Gibbs free energy departure	Normal
Vapor heat capacity	Normal
Vapor-Liquid K-value	Logarithmic
Vapor pressure	Logarithmic
Vapor thermal conductivity	Normal
Vapor viscosity	Normal
Vapor volume	Normal

† *If the model form is logarithmic, the tabular model uses the logarithmic transformation of the property to interpolate and extrapolate. The polynomial model is the logarithmic form of the equation.*

How Aspen Plus Uses Your Tabular Data and Polynomial Coefficients

Aspen Plus calculates the property for the component, using the tabular data and polynomial coefficients you enter. If you do not provide data for all components, Aspen Plus uses the property models of the ideal property method (IDEAL), for the components without data. For most properties, Aspen Plus calculates mixture properties using mole fraction average ideal mixing.

Aspen Plus uses your tabular data directly—Aspen Plus does not fit a polynomial equation to the data. When necessary, Aspen Plus uses a quadratic interpolation method to determine the property value at a given temperature. You should provide tabular data at small temperature intervals.

When the temperature is outside the lowest or highest temperature data that you entered, Aspen Plus calculates the property by linear extrapolation. If the model form is logarithmic, Aspen Plus uses the logarithmic transformation of the property to interpolate and extrapolate. For polynomial models when temperature is outside the lower and upper limits of the correlation, Aspen Plus also calculates the property by linear extrapolation.

If you enter	Then
Enthalpy or heat capacity data	You can use the Data Generation Options on the Specifications sheet to generate entropy and Gibbs free energy.
Vapor enthalpy data	Also enter ideal gas enthalpy data to ensure consistency.
Enthalpy, entropy, and Gibbs free energy	Make sure they are consistent (G = H – TS).

To enter experimental data for use with Property Estimation or Data Regression, use the Properties Data forms. For information on entering data for use in estimation or regression, see Chapters 30 and 31.

Entering Tabular Data

To enter tabular data:

1. From the Data menu, click Properties.
2. From the left pane of the Data Browser, go to the Properties Advanced Tabpoly Object Manager.
3. Click New to create a new object.
4. Enter an ID or accept the default ID, and then click OK.
5. On the Specifications sheet, choose the property for which you are entering data in the Property list. You can enter data for only one property on each Tabpoly form. Use as many forms as needed to enter your data.
6. In the For Property Method list, choose the property method for which the Tabpoly property is to be used. Specify All to use the data for all property methods in the simulation.
7. On the Data sheet, choose the component for which you have data, from the Component list box.
8. Select data type tabular Data, then enter the tabular data (property versus temperature) for the component.

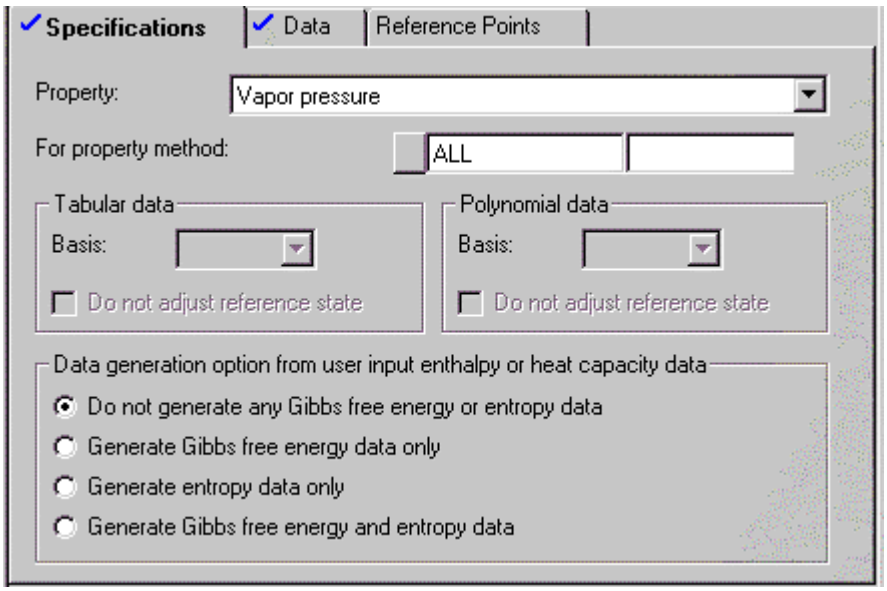
   You must enter the temperature-dependent tabular data in order of ascending temperature points. Aspen Plus determines the units for the temperature and the property data from the Units-Set you specify in the Units list box on the Data Browser toolbar.

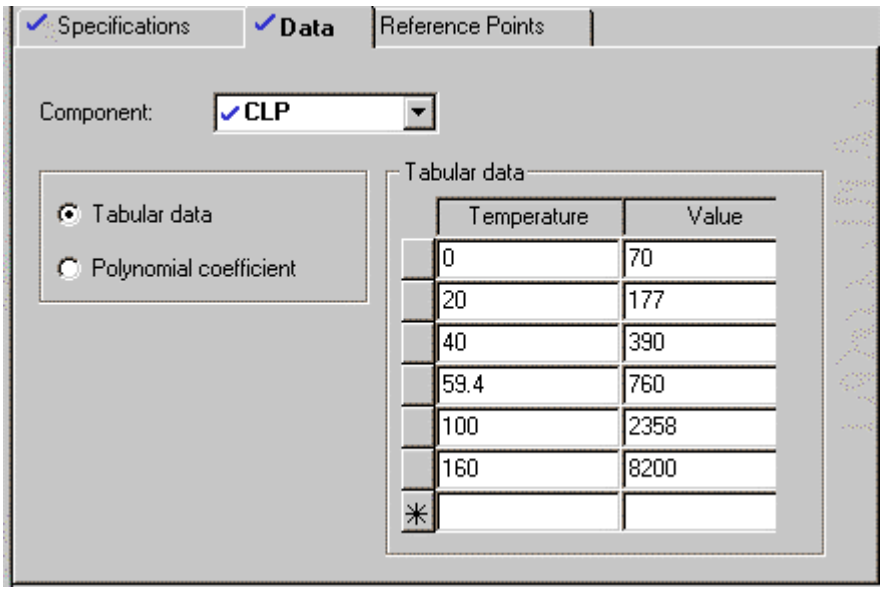
Example of Entering Vapor Pressure Data for Component CLP

This example assumes that the Units list box on the Data Browser toolbar is referencing a new Units-Set defined with temperature units of C and pressure units of mmHg.

Enter the following tabular data:

Vapor pressure (mmHg)	Temperature (C)
70	0
177	20
390	40
760	59.4
2358	100
8200	160





Entering Polynomial Coefficients for the General Polynomial Model

To enter polynomial coefficients for a general polynomial model:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser, double-click the Advanced folder.
3. Click the Tabpoly folder.
4. On the Tabpoly Object Manager, click New to create a new object.
5. Enter an ID or accept the default ID, and then click OK.
6. On the Specifications sheet, specify the property for which you are entering polynomial coefficients in the Property list box. You can enter polynomial coefficients for only one property on each form. Use as many forms as needed to enter your coefficients.
7. In the For Property Method list box, choose the property method for which the Tabpoly property is to be used. Specify All to use the data for all property methods in the simulation.
8. On the Data sheet, choose the component for which you have coefficients, from the Component list.
9. Select the data type: Polynomial Coefficient, then enter the general polynomial coefficients for the selected component.

   The polynomial model is of the form:

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

   See the Tabpoly Properties table on page 8-24 to determine whether the property you want to enter uses the normal or logarithmic form.

   The coefficients a_2 through a_8 default to zero. The lower temperature limit of the correlation (Min. temperature) defaults to 0 K. The upper temperature limit (Max. temperature) defaults to 1000 K. When the temperature is outside the limits, Aspen Plus calculates the property by linear extrapolation.

   The Units-Set you specify in the Units list box on the Data Browser toolbar determines the units for the coefficient values. If a_5, a_6, a_7, or a_8 is non-zero, Aspen Plus assumes absolute temperature units for all parameters.

Adjusting Reference States for Tabular Data and Polynomials

Aspen Plus can adjust the reference state of the enthalpy, entropy, and Gibbs free energy data that you entered. To specify this:

1. On the Tabpoly Specifications sheet, deselect the Do Not Adjust Reference State check box for your Tabular data or your Polynomial data.
2. Specify the basis (Mole or Mass) for your reference value and for the data, in the Basis list box.
3. On the Reference Points sheet, select the component for which you want to adjust the reference state, in the Component list box.
4. In the Reference Points boxes enter a reference Temperature and a reference value for Enthalpy, Entropy, or Gibbs free energy.
5. If you want to enter reference values and have Aspen Plus generate entropy and Gibbs free energy data from the enthalpy or heat capacity data that you enter, you must enter reference values for two of the three properties. The reference values are at the same temperature.
6. To use the Aspen Plus default reference state, do not enter any data on the Reference Points sheet. However, you must supply these parameter values for (or they must be available in the databanks):
   - DHFORM, DGFORM, PLXANT
   - DHVLWT (or DHVLDP)

   The Aspen Plus thermodynamic reference state is the component's constituent elements in an ideal gas state at 25°C and 1 atm.

If a simulation has	Then
No chemical reactions	You can select the reference states arbitrarily.
Chemical reactions	You must select reference states that include DHFORM for all components undergoing reaction.
Equilibrium reactions	You must select reference states that include DGFORM for all components undergoing reaction.

Adjusting Tabular Data or Polynomials for the Effect of Pressure

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

$$K(T,P) = \left(\frac{P_{ref}}{P}\right) K(T,P_{ref})$$

$$s(T,P) = s(T,P_{ref}) - R1n\left(\frac{P_{ref}}{P}\right)$$

$$g(T,P) = g(T,P_{ref}) - RT1n\left(\frac{P_{ref}}{P}\right)$$

Where:

P_{ref}	=	Reference pressure (the pressure at which the data was obtained.)
P	=	Actual system pressure
T	=	Temperature
$K(T,P_{ref})$	=	K-value at T and the reference pressure
$s(T,P_{ref})$	=	Entropy at T and the reference pressure
$g(T,P_{ref})$	=	Gibbs free energy at T and the reference pressure

Requesting Pressure Adjustment

To request pressure adjustment:

1. Go to the Reference Points sheet of the Tabpoly form.
2. Choose the component for which you want to specify the reference pressure, from the Component list box.
3. In the Pressure box, enter the reference pressure.

For K-values, Aspen Plus makes no adjustment for the pressure effect, unless you supply the reference pressure. You should always enter a reference pressure, unless the pressure range of the simulation matches that of the data.

If you use the Aspen Plus thermodynamic reference state for entropy and Gibbs free energy, an adjustment for the pressure effect is always performed using P_{ref} = 101325 N/m2. If you do not use the Aspen Plus reference state, Aspen Plus adjusts for the pressure effect only if you supply the reference pressure.

Using Property Data Packages

This section describes the Property Data Packages available in Aspen Plus.

You can use these data packages to model many important industrial processes. Theses data packages have been developed using publicly available literature data. They will be updated as new data becomes available. For your particular process, you may need to add or remove components and provide additional interaction parameters.

- Ammonia-water
- Ethylene
- Flue gas treatment
- Formaldehyde-methanol-water
- Glycol dehydration of natural gas
- Mineral solubilities in water using the Pitzer model
- Gas treating processes using amines: MDEA, DEA, DGA, AMP and MEA
- Methyl-amine

Using a Data Package

To use a data package:

1. From the File menu, click Import.
2. In the Import dialog box, click the Look In Favorites button.
3. From the list of favorite folders, select Data Packages.
4. Select the data package that you want and click Open.

Ammonia-Water Data Package

Use this data package for ammonia and water. This data package uses the Electrolyte NRTL model.

This data package is applicable from 5 - 250 C with pressure up to 100 bar.

Ethylene Data Package

Use this data package to model Ethylene processes. This data package uses the SR-POLAR equation of state model because of its versatility in representing both hydrocarbons and polar components such as water.

Pure component parameters were evaluated using experimental data for vapor pressure, liquid heat capacity and liquid density.

Binary parameters were evaluated from experimental VLE and LLE data.

This data package should provide a very good starting point for building the Ethylene process model. Simulation results can be improved by regressing missing binary parameters or updating the existing parameters with the new ones based on latest experimental data.

Using Electrolyte Amines Data Packages

Aspen Plus provides special data packages (inserts) for amines systems: MDEA, DEA, MEA, DGA and AMP (2-amino-2-methyl-1-propanol, C4H11NO-1).

These packages allow you to accurately model amines gas treating processes.

These inserts use the electrolyte capabilities, but also take into consideration kinetic reactions of CO2 in the liquid phase. The reaction kinetics can be used in either the RADFRAC or RATEFRAC distillation models. This modeling approach is fundamentally sound and has been validated through industrial applications. These data packages give more accurate results than those that do not consider kinetics reactions.

The following table shows the range of applications:

System	Insert Name	Temperature	Amines Concentration
AMP	KEAMP	40-100 C	2.47 to 4.44 molal
MDEA	KEMDEA	25 - 120 C	Up to 50 weight %
DEA	KEDEA	Up to 140 C	Up to 30 weight %
DGA	KEDGA	Up to 100 C	Up to 65 weight %
MEA	KEMEA	Up to 120 C	Up to 50 weight %

Using an Amines Data Package

To use an amines insert:

1. From the File menu, click Import.
2. In the Import dialog box, click the Look In Favorites button.
3. From the list of favorite folders, select Data Packages.
4. Select the desired data package and click Open.
5. In the Parameter Values dialog box, enter the component IDs you are using for the amine, CO2 and H2S by first selecting the Parameter then clicking the Edit Value button.

   Make sure that you use the true component approach on the Properties Specifications Global sheet or the Block Options Properties sheet of a unit operation model. This is required for all the amines data packages that use kinetic reactions.
6. If you are using RADFRAC or RATEFRAC, specify one of the following Reaction IDs on the Reactions form for the model:

Reaction ID	For modeling	When using this data package
MDEA-CO2	CO2 absorption	KEMDEA
MDEA-ACID	CO2/H2S absorption	KEMDEA
MEA-CO2	CO2 absorption	KEMEA
MEA-ACID	CO2/H2S absorption	KEMEA
DEA-CO2	CO2 absorption	KEDEA
DEA-ACID	CO2/H2S absorption	KEDEA

Flue Gas Treatment Data Package

Use this data package to model flue-gas purification process. The data package uses the Electrolyte NRTL model.

The apparent components are:

H2O, N2, O2, CO2, CO, SO2, SO3, NO, NO2, HCL, HF, HNO3, HNO2, H2SO4, H2SEO3, HGCL2, HG2CL2, HG, C, SE, SEO2, HG(OH)2, CASO4*2W, CAF2, CAO, CA(OH)2

The Henry-components are:

CO CO2 SO2 HCL O2 N2 NO HG

Valid temperature range from: 273.15 K to 373.15 K

Formaldehyde-Methanol-Water Data Package

Use this data package to model Formaldehyde-Methanol-Water system. This system is highly non-ideal because the three components form multiple complexes.

The vapor phase is modeled using the Hayden-O'Connell model. This model properly accounts for the strong association in the vapor phase.

The liquid phase is modeled using the UNIFAC model with special group-group interaction parameters determined from regression of experimental data. The complexes such as methylene glycol and hemiformal are formed using the Chemistry reactions.

Valid temperature range: 0 to 100 C

Mole fraction of Formaldehyde: 0 - 0.6

Pressure: 0 - 3 bar

Glycol Dehydration Data Package

Use this data package to model natural gas dehydration processes using glycols (Ethylene glycol (EG): C2H6O2, Di-ethylene glycol (DEG): C4H10O3, or Tri-ethylene glycol (TEG): C6H14O4)

The data package uses the Schwartzentruber-Renon equation-of-state (SR-POLAR) model.

The components included in this package are:

EG, DEG, TEG, WATER, METHANOL, CO2, N2, H2S, METHANE, ETHANE, PROPANE, N-BUTANE, N-PENTANE, N-HEXANE, N-HEPTANE, N-OCTANE, N-NONANE, N-DECANE, BENZENE, TOLUENE, O-XYLENE, ISO-BUTANE, ISO-PENTANE, ETHYLENE, PROPYLENE

The experimental data used to develop the data package cover very wide range of temperatures and pressures.

Pitzer Data Packages

There are four data packages for calculating mineral solubilities in water using the Pitzer electrolyte model:

1. PITZ_1: for prediction of mineral solubilities in water at 25 C. The system is Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O.
2. PITZ_2: for prediction of mineral solubilities in water for systems:

   Na-K-Ca-Ba-Cl-H2O and Na-Ca-Cl-SO4-H2O.

   The apparent components are:

   H2O, NACL, KCL, CACL2, ACL2*4H2O, CACL2*6H2O, BACL2, ACL2*2H2O

   Valid temperature range: up to 200 C

   Valid pressure: equilibrium to 1 atmosphere
3. PITZ_3: for Na-K-Ca-Cl-SO4-NO3-H2O system

   The apparent components are:

   H2O, NA2SO4, NACL, NA2SO4*10H2O, NA2CA(SO4)2, NA4CA(SO4)3*2H2O, NANO3, K2SO4, KCL, K2CA(SO4)2*H2O, KNO3, CACL2, CASO4, CACL2, CACL2*6H2O, CASO4*2H2O, 2(CASO4)**H2O, CACL2*4H2O,CA(NO3)2, CA(NO3)2*4H2O

   Valid temperature range: 0 - 250 C
4. PITZ_4 for H2O- NaCl- Na2SO4- KCl- K2SO4- CaCl2- CaSO4- MgCl2- MgSO4- CaCl2*6H2O- MgCl2*6H2O- MgCl2*8H2O- MgCl2*12H2O- KMgCl3*6H2O- Mg2CaCl6*12H2O- Na2SO4*10H2O- MgSO4*6H2O- MgSO4*7H2O- K2Mg(SO4)2*6H2O

   Valid temperature range : -60 to 25 C

Methyl-amine Data Package

Use this data package to model methyl-amines process. This system is highly non-ideal. The components included are: ammonia, water, methanol, methyl-amine, dimethylamine and trimethyl-amine.

The property model used for representing VLE data is the SR-POLAR equation of state. High pressure VLE data for NH3-H2O and Methanol-Water were used in the regression. This model is particularly good for high pressure column. The results may be improved by adding additional binary parameters for the EOS based on new VLE data.

Pure component parameters were evaluated using liquid Density, Heat Capacity and Vapor pressure data.

Using Other Electrolyte Data Packages

The following tables show electrolyte data packages that are available in the ELECINS sub-directory.

This table shows electrolyte data packages, available in the ELECINS sub-directory, that use the ELECNRTL property method:

Property Method ELECNRTL

Filename	Electrolyte System
h2ohc.bkp	H2O - HCL (as Henry-comps)
ehno3.bkp	H2O - HNO3
enaoh.bkp	H2O - NAOH
eso4br.bkp	H2O - H2SO4 - HBR
ehbr.bkp	H2O - HBR
ehi.bkp	H2O - HI
eh2so4.bkp	H2O - H2SO4
ehclmg.bkp	H2O - HCL - MGCL2
enaohs.bkp	H2O - NAOH - SO2
eso4cl.bkp	H2O - H2SO4 - HCL
ecauts.bkp	H2O - NAOH - NACL - NA2SO4 -NA2SO4.10H2O -NA2SO4.NAOH - NA2SO4.NAOH.NACL
ekoh.bkp	H2O - KOH
ecaust.bkp	H2O - NAOH - NACL - NA2SO4
ehcl.bkp	H2O - HCL (as solvent)
ehclle.bkp	H2O - HCL (as solvent, recommend for LLE)
edea.bkp	H2O - DEA - H2S - CO2
ehotde.bkp	H2O - DEA - K2CO3 - H2S - CO2
emea.bkp	H2O - MEA - H2S - CO2
ecl2.bkp	H2O - CL2 - HCL
enh3co.bkp	H2O - NH3 - CO2
enh3so.bkp	H2O - NH3 - SO2
esouro.bkp	H2O - NH3 - H2S - CO2 - NAOH
edga.bkp	H2O - DGA - H2S - CO2
enh3h2.bkp	H2O - NH3 - H2S
eamp.bkp	H2O - AMP - H2S - CO2
ehotca.bkp	H2O - K2CO3 - CO2

Continued

Filename	Electrolyte System
enh3hc.bkp	H2O - NH3 - HCN
ebrine.bkp	H2O - CO2 - H2S - NACL
ebrinx.bkp	H2O - CO2 - H2S - NACL (extended Temperature range)
eclscr.bkp	H2O - CL2 - CO2 - HCL - NAOH - NACL - NA2CO3
ekohx.bkp	H2O - KOH (high concentration)
ehf.bkp	H2O - HF
ehotcb.bkp	H2O - K2CO3 - CO2 - KHCO3
emdea.bkp	H2O - MDEA - CO2 - H2S
enh3po.bkp	H2O - NH3 - H3PO4 - H2S
esour.bkp	H2O - NH3 - H2S - CO2

This table shows electrolyte data packages, available in the ELECINS sub-directory, that use the SYSOP15M property method:

Property Method SYSOP15M

Filename	Electrolyte System
brine.bkp	H2O - CO2 - H2S - NACL
caust.bkp	H2O - NAOH - NACL - NA2SO4
causts.bkp	H2O - NAOH - NACL - NA2SO4 -NA2SO4.10H2O -NA2SO4.NAOH - NA2SO4.NAOH.NACL
dea.bkp	H2O - DEA - H2S - CO2
dga.bkp	H2O - DGA - H2S - CO2
h2ohbr.bkp	H2O - HBR
h2ohcl.bkp	H2O - HCL
h2ohf.bkp	H2O - HF
h2ohi.bkp	H2O - HI
hotca.bkp	H2O - K2CO3 - CO2
hotcb.bkp	H2O - K2CO3 - CO2 - KHCO3
hotdea.bkp	H2O - DEA - K2CO3 - H2S - CO2
mcl2.bkp	H2O - CL2
mdea.bkp	H2O - MDEA - H2S - CO2
mea.bkp	H2O - MEA - H2S - CO2
mh2so4.bkp	H2O - H2SO4
mhbr.bkp	H2O - HBR

Continued

Filename	Electrolyte System
mhcl.bkp	H2O - HCL
mhcl1.bkp	H2O - HCL
mhclmg.bkp	H2O - HCL - MGCL2
mhf.bkp	H2O - HF
mhf2.bkp	H2O - HF (to 100% HF)
mhno3.bkp	H2O - HNO3
mnaoh.bkp	H2O - NAOH
mnaoh1.bkp	H2O - NAOH
mso4br.bkp	H2O - H2SO4 - HBR
mso4cl.bkp	H2O - H2SO4 - HCL
naohso.bkp	H2O - NAOH - SO2
nh3co2.bkp	H2O - NH3 - CO2
nh3h2s.bkp	H2O - NH3 - H2S
nh3hcn.bkp	H2O - HCN
nh3po4.bkp	H2O - NH3 - H2S - H3PO4
nh3so2.bkp	H2O - NH3 - SO2
sour.bkp	H2O - NH3 - H2S - CO2
souroh.bkp	H2O - NH3 - H2S - CO2 - NAOH

This table shows electrolyte data packages, available in the ELECINS sub-directory, that use the SYSOP16 property method:

Property Method SYSOP16

Filename	Electrolyte System
pnh3co.bkp	H2O - NH3 - CO2
pnh3h2.bkp	H2O - NH3
pnh3so.bkp	H2O - NH3 - SO2
psour.bkp	H2O - NH3 - H2S - CO2

❖ ❖ ❖ ❖

9 Specifying Streams

Streams connect unit operation blocks in a flowsheet and carry material and energy flow from one block to another. Streams can be:

- Feed streams to the flowsheet
- Internal (interconnecting) streams within the flowsheet
- Product streams from the flowsheet
- Pseudo-product streams representing flows internal to a block

Use the Stream forms to enter data for the feed streams and to give initial estimates for any internal streams that are tear (recycle) streams.

This chapter includes information about:

- Specifying material streams
- Analyzing stream properties interactively
- Specifying stream classes and substreams
- About particle size distributions
- Accessing stream libraries
- Specifying work streams
- Specifying heat streams
- Using pseudoproduct streams

Specifying Material Streams

For all material process feed streams, you must specify:

- Flow rate
- Composition
- Thermodynamic condition

You can provide initial guesses of these variables for tear (recycle) streams.

Entering Specifications for Streams

To enter specifications for a stream:

1. Double-click the stream in the flowsheet.

   – or –

   From the Data menu, click Streams. In the Streams Object Manager, select the stream and click Edit.

2. On the Specifications sheet, specify any two of three State Variables to set the thermodynamic condition of your stream. For example, you could specify temperature and pressure, or temperature and vapor fraction. For the available options, see Possible Stream Thermodynamic Condition Specifications on page 9-3.
3. Specify the stream composition using flow rates or flow fractions or flow concentrations of each component in the Composition frame. See Entering Stream Composition on page 9-4.

   Perform Steps 4 through 6 only if the stream contains solids substreams.

4. If you want to specify solids substreams, use the Substream field to display different substreams.
5. Specify temperature, pressure, and composition for each solids substream. You must specify the same pressure for each substream.
6. If any components in the stream have component attributes, or any substreams have particle size distributions, you must specify values for them. For more information, see Specifying Particle Size Distribution

To specify the particle size distribution for a solid substream:

1. Double-click the stream in the flowsheet

   – or –

   From the Data menu, click Streams. In the Streams Object Manager select the stream and click the Edit button.

2. On the Stream Input form, click the Stream PSD sheet.
3. Enter the weight fractions for the particle sizes. The total should be 1.0.

   For more information about particle size distribution in Aspen Plus, and how to define your own particle size ranges, see Defining New Substreams on page 9-20.

7. Specifying Component Attribute Values on page 9-7 and Specifying Particle Size Distribution on page9-7.

Possible Stream Thermodynamic Condition Specifications

This table describes possible stream thermodynamic condition specifications:

Phases	Free Water	State Specification	Stream Properties Calculated by
Vapor only	No	Temperature, Pressure	Vapor phase thermodynamic calculations
Solid only	No	Temperature, Pressure	Solid phase thermodynamic calculations
Liquid only	No	Temperature, Pressure	Liquid phase thermodynamic calculations
Liquid-freewater	Yes	Temperature, Pressure	Liquid phase thermodynamic calculations with free water considered
Vapor-liquid or vapor-liquid-liquid	No	Temperature, Pressure	TP flash
Vapor-liquid or vapor-liquid-liquid	No	Temperature, Molar Vapor fraction	TV flash
Vapor-liquid or vapor-liquid-liquid	No	Pressure, Molar Vapor fraction	PV flash
Vapor-liquid-freewater	Yes	Temperature, Pressure	TP flash with free water considered
Vapor-liquid-freewater	Yes	Temperature, Molar Vapor fraction	TV flash with free water considered
Vapor-liquid-freewater	Yes	Pressure, Molar Vapor fraction	PV flash with free water considered

Aspen Plus calculates unspecified temperature, pressure, or molar vapor fraction, as well as the stream enthalpy, entropy, and density.

Mass-Balance-Only Calculations

If you are performing a mass-balance-only simulation:

1. Double-click the stream in the flowsheet

   – or –

   From the Data menu, click Streams. In the Streams Object Manager select the stream and click the Edit button.

2. Ensure the Calculate Stream Properties check box on the Stream Input Flash Options sheet is clear.
3. Enter values for two of the following: Temperature, Pressure, and Vapor fraction as State Variables on the Stream Input Specifications sheet.

For more information on checking mass balances around blocks, click here. See Chapter 5.

Aspen Plus does not calculate stream properties in mass-balance-only simulations.

Entering Stream Composition

You can specify the stream composition in terms of component flows, fractions, or concentrations.

For	Enter values on this basis
Component flows or fractions†	Mole, mass, or standard liquid volume
Concentrations	Mole or mass

† *For nonconventional components, you can enter only mass flows and fractions.*

If you specify component fractions, you must specify the total mole, mass, or standard liquid volume flow. Component fractions must sum to 1.0 or 100.0.

You can enter both component flows and total flow. Aspen Plus normalizes the component flows to match the total flow.

If you specify component concentrations, you must enter a component ID for the solvent and the total flow. The stream must be single phase. You can select Vapor-Only or Liquid-Only in the Valid Phases list on the Stream Input Flash Options sheet, and temperature and pressure as State Variables on the Stream Input Specifications sheet. Or you can specify the stream at its bubble point (Vapor Fraction is 0).

If you use the standard liquid volume basis for component flows, fractions or total stream flow, you need to enter the standard liquid volume of a component (VLSTD) on the Properties Parameters Pure Component Input form. For more information, see Chapter 8. The values for VLSTD in the databanks are from the API databook. The standard liquid volume is not used to calculate densities in Aspen Plus.

The standard liquid volume flow (Stdvol-Flow) can be very different from the volumetric flow rate of a stream. The standard liquid volume is defined at approximately 60ºF and 1 atm. The difference increases as the conditions diverge from 60ºF and 1 atm. If the stream is a vapor or has a significant amount of vapor, the volumetric flow rate of a stream is extremely different from the standard liquid volume flow. You can enter standard vapor volume flows as mole-flow. Select the appropriate units (for example scfm).

To report the Std.liq. Volume Flow or Std.liq.Volume Fraction in the stream report, select the appropriate options on the Setup ReportOptions Stream sheet. You can also calculate these Property Sets:

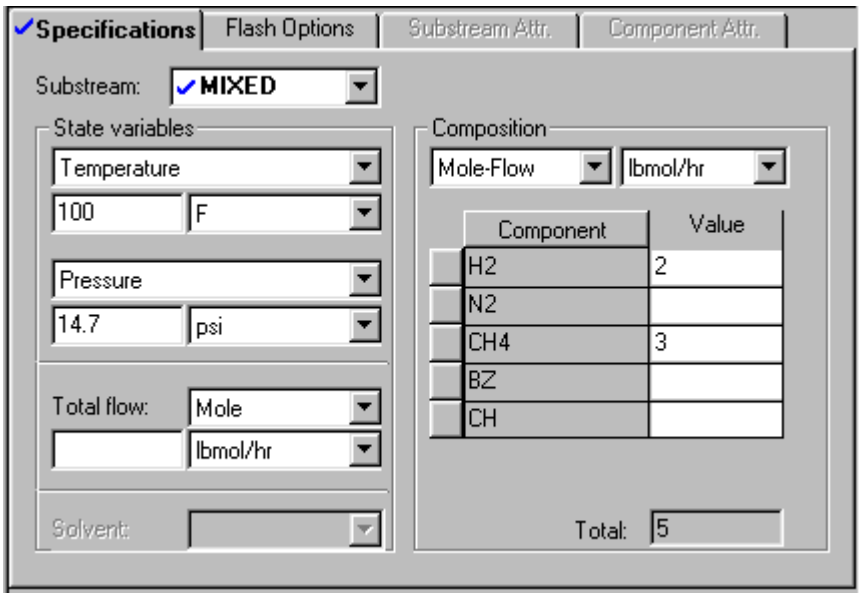
- VLSTDMX (standard liquid volume of a mixture)
- VLSTD (standard liquid volume of a component)

StdVol-Flow and StdVol-Frac are accessible variables that can be used in design specifications and Fortran blocks.

The Stream Input Specifications sheet displays the total of the component flows, fractions, or concentrations entered for the stream. Use this value to check your input.

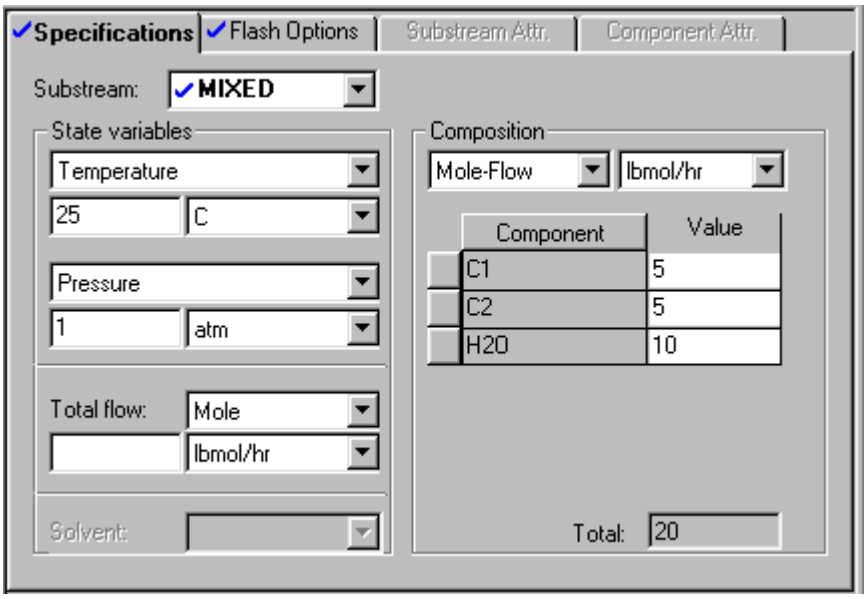
Example for Specifying a Process Feed Stream

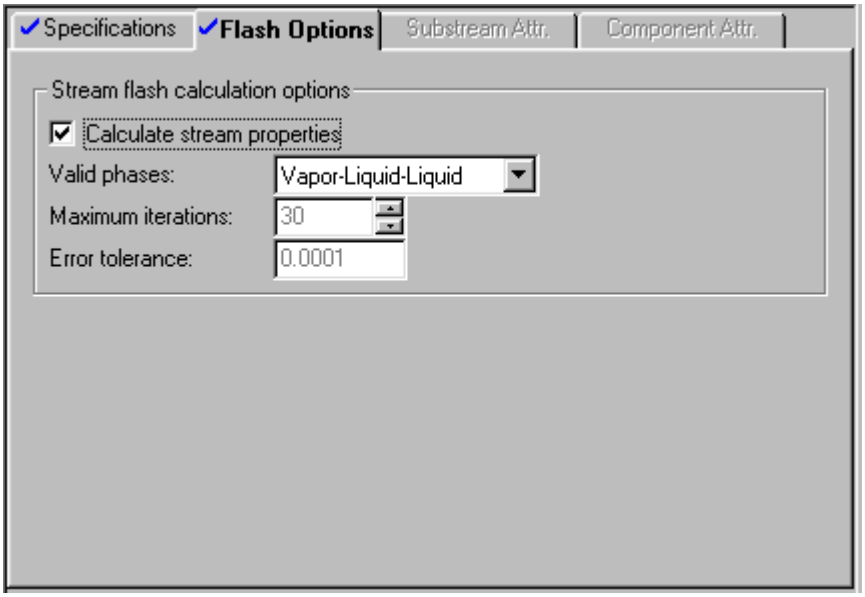
A process feed stream (FEED) contains 2 lbmol/hr of hydrogen (H2) and 3 lbmol/hr of methane (CH4), at 100F and 14.7 psia. Aspen Plus performs a two-phase flash to determine stream properties and phase conditions.



Example for Specifying a Stream with Two Liquid Phases

A process feed stream contains 5 lbmol/hr of C1, 5 lbmol/hr of C2, and 10 lbmol/hr of H2O. Two partially miscible liquid phases are anticipated. The vapor-liquid-liquid equilibrium is treated rigorously. Aspen Plus performs a three-phase flash to determine phase condition.





Specifying Particle Size Distribution

To specify the particle size distribution for a solid substream:

2. Double-click the stream in the flowsheet

   – or –

   From the Data menu, click Streams. In the Streams Object Manager select the stream and click the Edit button.

4. On the Stream Input form, click the Stream PSD sheet.
5. Enter the weight fractions for the particle sizes. The total should be 1.0.

   For more information about particle size distribution in Aspen Plus, and how to define your own particle size ranges, see Defining New Substreams on page 9-20.

Specifying Component Attribute Values

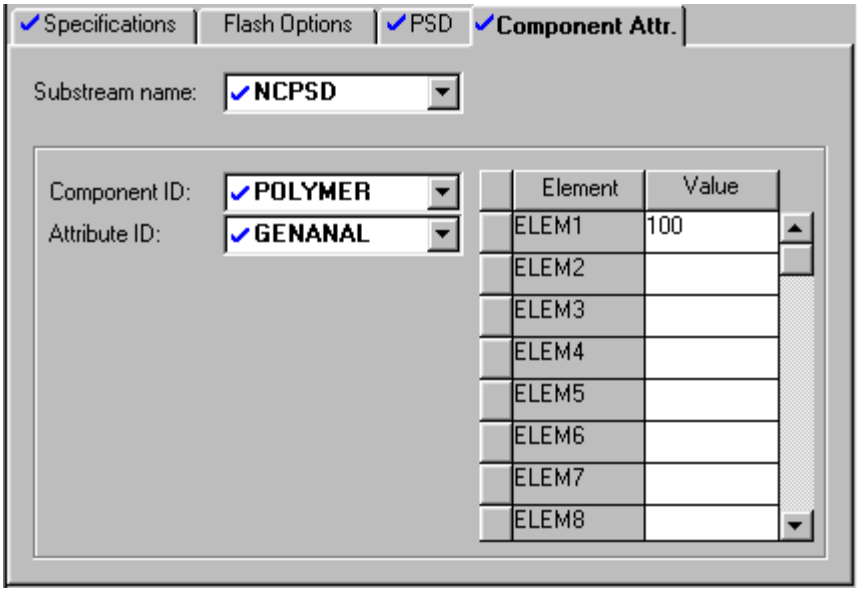
Use the Stream Input Component Attr. sheet to specify values of component attributes. You must specify values for each attribute defined on the Components Attr-Comps selection sheet or Properties Advanced NC-Props PropertyMethods sheet (see Chapter 5).

To specify values of component attributes for a stream:

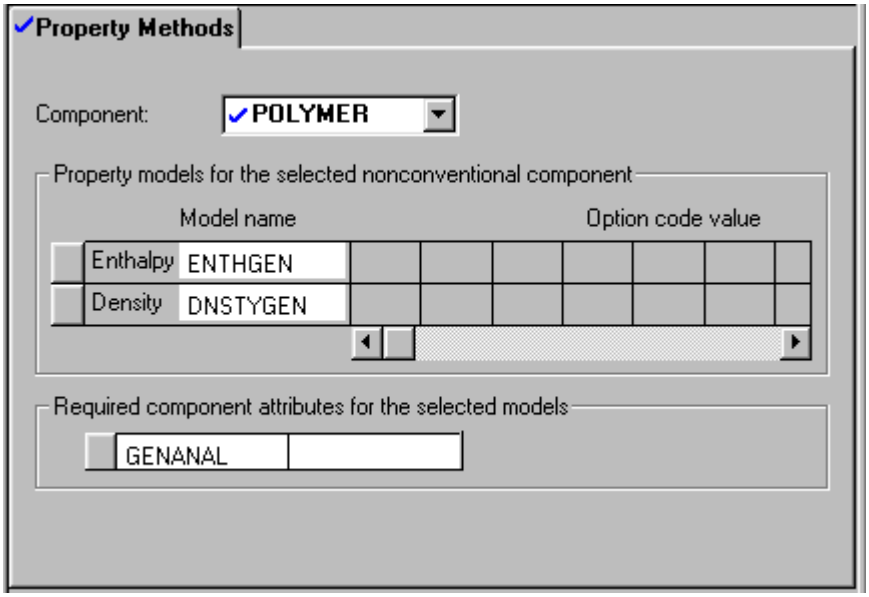
1. On the Stream Input form, click the Component Attr. sheet.
2. Enter values for each attribute listed.

Example of Specifying the GENANAL Component Attributes for a Nonconventional Substream

On the Stream Input Component Attr. sheet, the elements of the GENANAL component attribute are specified for the NCPSD substream.



On the Properties Advanced NC-Props form, the GENANAL component attribute is defined as required for the selected Nonconventional Component Property models.



About Stream Property Analysis

You can calculate and display stream properties interactively as you create your simulation model. You do not have to complete the flowsheet definition or input specifications first.

For example, you can flash a feed stream as soon as you define it, to check your property model. As you develop a flowsheet model interactively, you can check the phase behavior of intermediate streams to help you determine feasible specifications.

The following table shows the types of stream analysis you can perform:

Stream Analysis Types

Type	Description
Point	Stream properties for the total stream and each of the phases present. Properties include temperature, pressure, phase fractions, flow rate, heat capacity, density, and transport properties.
Component Flow	Component flow rates for the total stream and each of the phases present. Mole, mass, and standard volume fractions are available.
Composition	Component fractions for the total stream and each of the phases present. Mole, mass, and standard volume fractions are available. Partial pressure is also available.
Petroleum	Point properties, plus API gravity, specific gravity, Watson K factor, and kinematic viscosity
Dist-Curve†	Petroleum distillation curves (TBP, D86, D160, and vacuum)
Bubble/Dew††	Bubble point temperature and dew point temperature versus pressure curves
PV Curve††	Vapor fraction versus pressure curves at stream temperature
TV Curve††	Vapor fraction versus temperature curves at stream pressure
PT-Envelope††	Pressure-temperature envelope curves For more information, see Generating PT-Envelopes on page 913.

† *Plots can be generated from this analysis.*

†† *These analyses automatically display plots of the curves.*

You can also perform stream property analyses using property tables. The Analysis commands automate many of the steps required to generate a property table, and define built-in plots appropriate for the analysis.

Use the Property Table forms when you need flexibility not provided by the Analysis commands.

Analyzing Stream Properties

To calculate and display stream properties interactively:

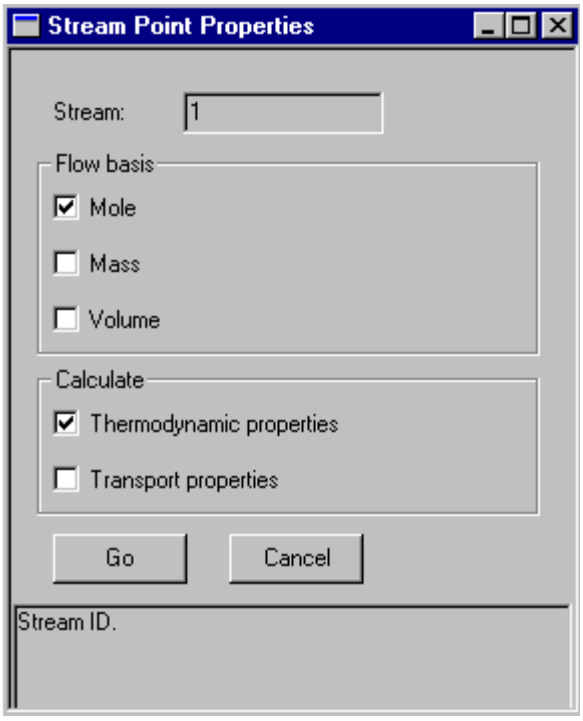
1. Make sure your Setup, Components, and Properties specifications are complete.
2. Make sure the specifications or results for the stream you want to analyze are complete. Either the Stream Input Specifications sheet for the stream must be complete or the stream must have results that were calculated in the current session.
3. Click the stream to select it.
4. On the Tools menu, point to Analysis, then Stream, then choose the type of calculation you want to perform.

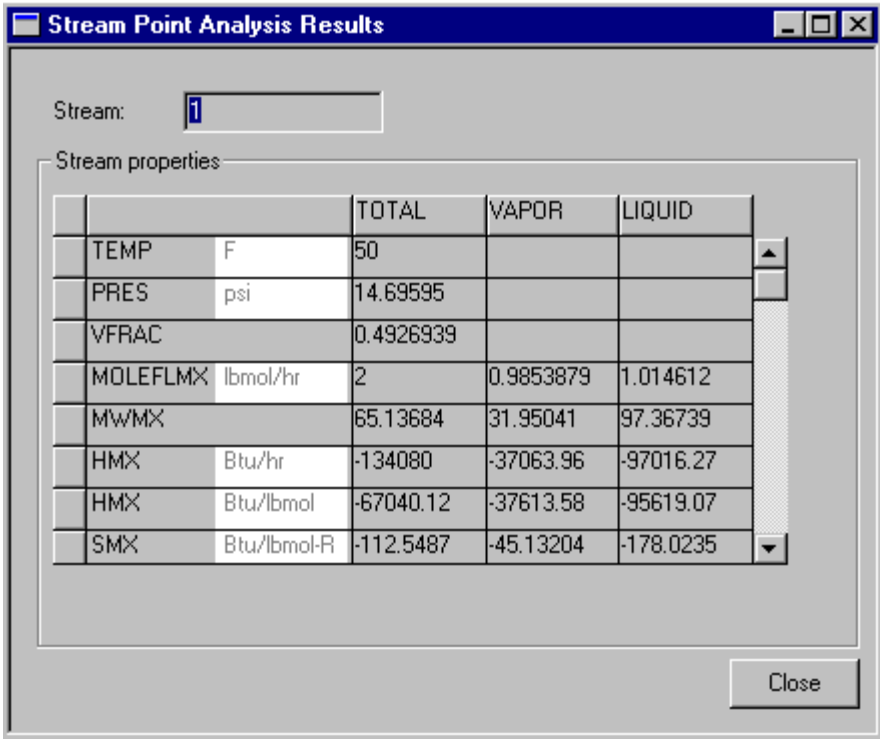
   This command will be inactive if the conditions in Steps 1 and 2 are not satisfied.
5. Make any selections and specifications you want in the appropriate dialog box.

   If you selected Bubble/Dew or PV curve, you must specify a pressure range. If you selected TV curve, you must specify a temperature range.
6. Click Go.
7. Print or view results and plots that appear when calculations are complete.
8. Close the form and plot when you are sure you are finished with the results. ***The results are not saved.*** You must redo the calculations if you want to look at them again, once you close the form.

Example of Generating Point Analysis of a Stream

Stream 1 is a 50-50 mixture of ethane and heptane.

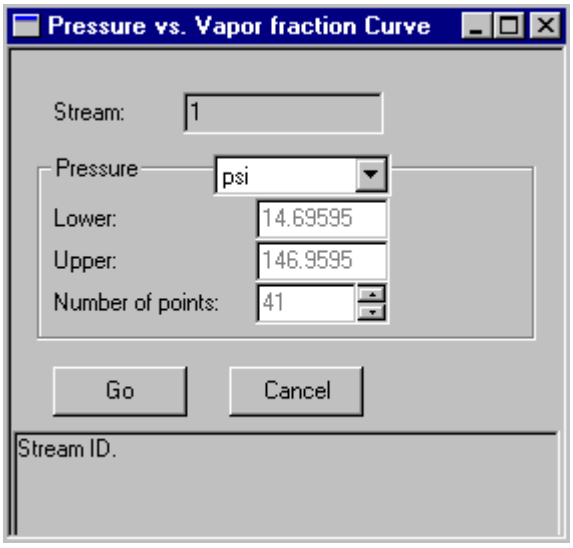


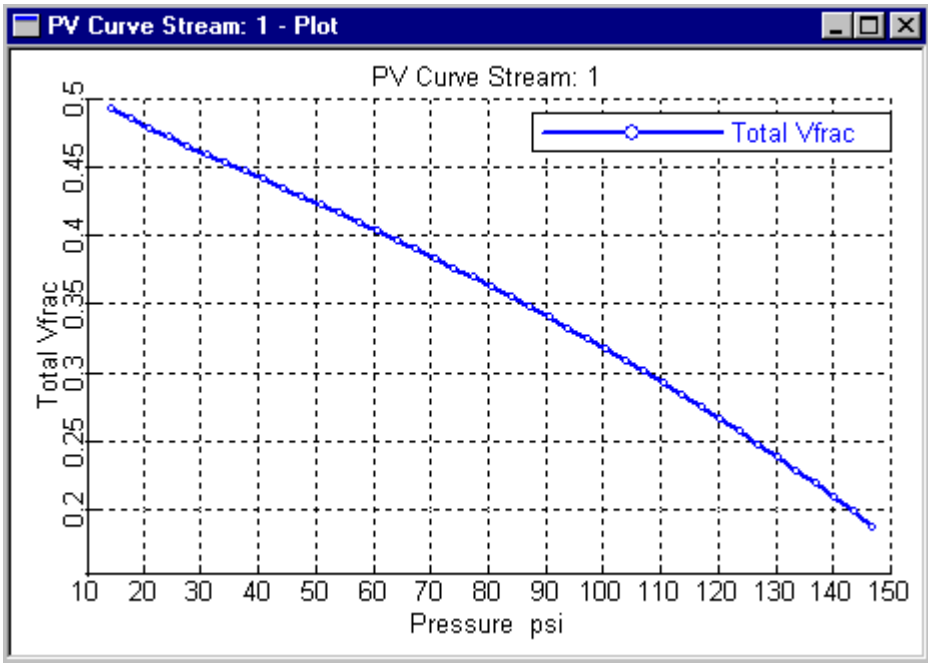


Example of Generating PV Curve

Stream 1 is a 50-50 mixture of ethane and heptane.

Stream Temperature is 270 F.





Generating PT-Envelopes

Pressure-temperature (PT) envelopes are generated by following curves of constant vapor fraction, through the critical point and back out the complementary branch. (The complementary branch for Vapor fraction = 0.75 is 0.25.) These plots are parametric, consisting of one curve for each vapor fraction and its complementary branch.

You can generate PT-Envelopes from any property method, except electrolyte property methods. But PT-Envelopes generated from activity coefficient-based and other non-equation-of-state property methods will not pass through the critical point. Instead there will be separate curves for each vapor fraction and its complementary branch.

For more information about PT-envelopes, see Chapter 27.

Creating a PT-Envelope from a Stream

To create a PT-Envelope from a stream:

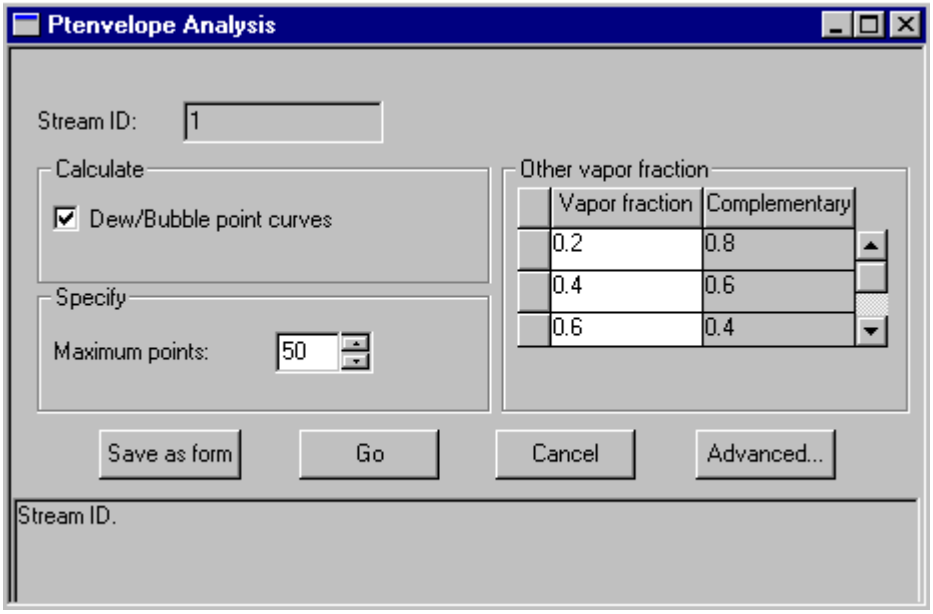
1. Make sure your Setup, Components, and Properties specifications are complete.
2. Make sure the specifications or results for the stream you want to analyze are complete. Either the Stream Input Specifications sheet for the stream must be complete or the stream must have results that were calculated in the current session.
3. Click the stream to select it.
4. From the Tools menu, point to Analysis, then Stream. This command will be inactive if the conditions in Steps 1 and 2 are not satisfied.
5. Choose PT-Envelope.
6. Select the vapor fraction branches.

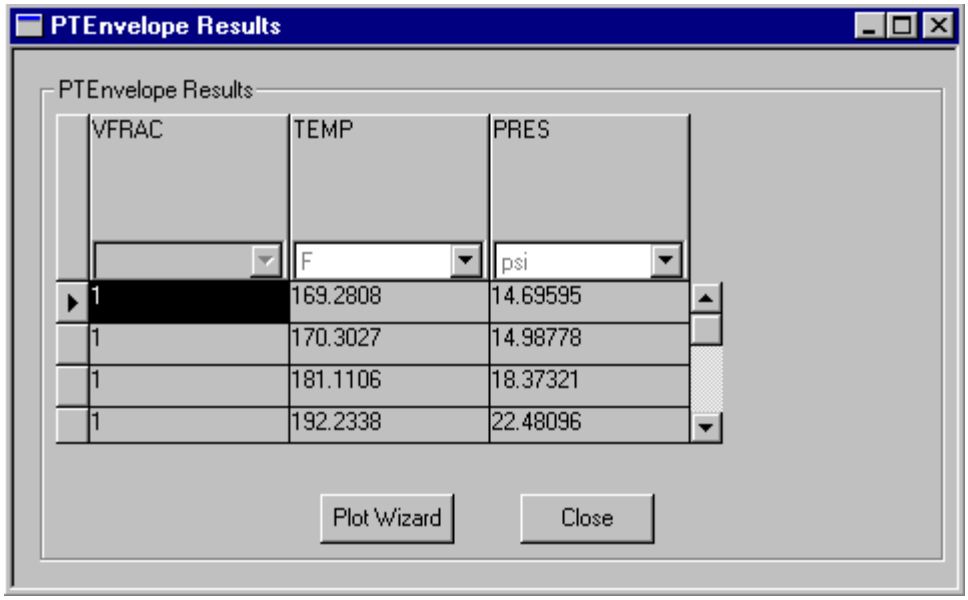
   The Dew/Bubble point curves correspond to vapor fractions of 0 and 1.0. Additional vapor fractions can be specified. The complementary vapor fraction is automatically calculated for each vapor fraction specified.
7. Click Go to create the PT-Envelope table and plot. For more information on customizing the plot, see Chapter 13.

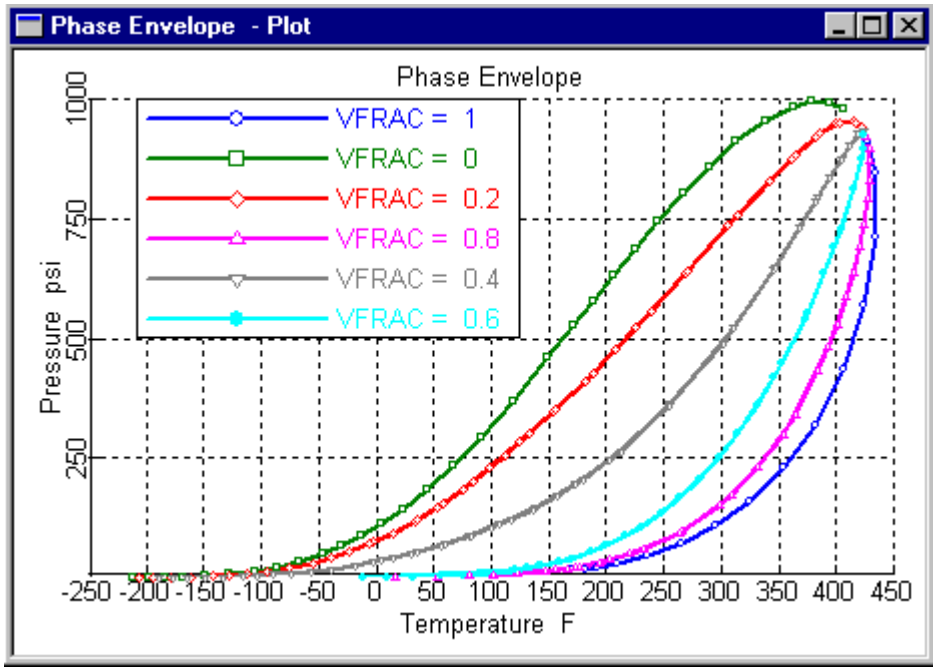
8. Close the form and plot when you are sure you are finished with the results. ***The results are not saved.*** You must redo the calculations if you want to look at them again, once you close the form. To save the input and the table of results, click the Save as Form button before closing the PT-Envelope Analysis form and the a form with the input and results will be saved in the Property Analysis folder.

Example of Creating a PT Envelope

For example, a table of values and a plot for a P-T envelope is generated for vapor fractions of 0.0, 0.2, 0.4, 0.6, 0.8, and 1.0 for a 50-50 mixture of ethane and heptane in stream 2.




PTEnvelope Results
PTEnvelope Results
VFRAC
TEMP
PRES
F
psi
1 169.2808 14.69595
1 170.3027 14.98778
1 181.1106 18.37321
1 192.2338 22.48096
Plot Wizard
Close


Phase Envelope - Plot
Phase Envelope
VFRAC = 1
VFRAC = 0
VFRAC = 0.2
VFRAC = 0.8
VFRAC = 0.4
VFRAC = 0.6
Pressure psi
1000
750
500
250
-250 -200 -150 -100 -50 0 50 100 150 200 250 300 350 400 450
Temperature F

About Stream Classes

You do not need to specify stream classes if:

- Your simulation does not involve solids
- The only solids are electrolytes salts defined using Chemistry forms or the Electrolytes Expert System

Stream classes define structures for simulation streams when solids are present. Solids are:

- Carried in substreams
- Characterized as either conventional or nonconventional components. For more information, see Chapter 6.
- May have a particle size distribution (PSD)

A stream class defines a stream structure in terms of:

- Number of substreams
- Type of component carried in each substream (conventional or nonconventional)
- Whether the substream carries particle size distribution information

Use this Setup StreamClass sheet	To
Flowsheet	Assign a new Stream Class to a flowsheet section, and define the substreams in a stream class
Streams	Assign streams to a stream class, and define the substreams in a stream class

Use the Stream Input PSD sheet to define the particle size distribution weight fractions for a substream.

The following sections describe how you can:For help on using Stream Classes, click one of the following topics:

- Use predefined stream classes
- Create your own stream classes
- Assign stream classes globally
- Assign stream classes to flowsheet sections
- Assign stream classes to individual streams

Using Predefined Stream Classes

These stream classes are predefined in Aspen Plus and should be sufficient for most applications:

Use this stream class	When
CONVEN	The simulation does not involve solids, or the only solids are electrolytes salts.
MIXCISLD	Conventional solids are present, but there is no particle size distribution.
MIXNC	Nonconventional solids are present, but there is no particle size distribution.
MIXCINC	Both conventional and nonconventional solids are present, but there is no particle size distribution.
MIXCIPSD	Conventional solids are present, with a particle size distribution.
MIXNCPSD	Nonconventional solids are present, with a particle size distribution.

All unit operation models (except Extract) can handle stream classes with solid substreams:

These models	Require
All except Mixer and ClChng	All inlet and outlet streams belonging to the same stream class
CFuge, Filter, SWash, CCD	At least one solids substream
Crusher, Screen, FabFl, Cyclone, VScrub, ESP, HyCyc	At least one solids substream with a particle size distribution
Crystallizer	At least one solids substream with a particle size distribution, if particle sizes are calculated

You can also assign stream classes globally, or to flowsheet sections or individual streams.

Creating or Modifying Stream Classes

You need to create or modify a stream class to:

- Add new substreams to a stream class
- Create a stream class with PSD attributes for both CISOLID and NC type substreams
- Use two or more particle size distribution definitions in a simulation

The number and types of substreams, together with their attributes, define a stream class. A stream class can have any number of substreams but the first substream for each Stream Class must be of type MIXED.

Each substream:

- Must be assigned a type (MIXED, CISOLID, or NC)
- Can be assigned a particle size distribution (PSD)

You can create a new stream class by listing all its substreams, or you can modify the substreams in an existing stream class. You cannot modify a MIXED type substream.

Use the Define StreamClass button on the Flowsheet or Streams sheet of the Setup StreamClass form, to assign a new stream class to the structure of a stream by listing its constituent substreams or to modify the substreams in an existing stream class.

To create or modify a substream:

1. From the Data menu, click Setup.
2. In the left pane of the Data Browser, select the Setup Stream Class form.
3. On the Flowsheet sheet, click the Define StreamClass button.
4. On the Define StreamClass dialog box, select <new> from the list in the Stream Class field.

   –or–

   Use the list in the StreamClass box to select the name of the Stream Class to be modified.
5. Select the substreams to include in the stream class from the Available substreams list and use the right arrow button to move them into the Selected substreams list. The left arrow can be used to remove substreams from the Selected substream list. The double arrow can be used to move all of the substreams in a list at one time.
6. Use the up and down arrow buttons to rearrange the list. Note that the first substream must be of type MIXED.
7. When finished, on the Define StreamClass dialog box, click Close.

Specifying a Global Stream Class

You can specify the default stream class globallyfor all streams in a simulation. You can override the global default for a flowsheet section or for an individual stream.

The default stream class is the stream class for flowsheet section GLOBAL. The default stream class is established by the Application Type you choose when creating a new run. You can change this default on the Setup Specifications Global sheet.

To specify the default stream class using the Setup Specifications Global sheet:

1. From the Data menu, click Setup.
2. In the left pane of the Data Browser, click the Specifications folder.
3. On the Global sheet, select a stream class in the Stream Class field.

Specifying Stream Classes for Flowsheet Sections

When using more than one stream class in a simulation, divide the flowsheet into sections and specify a stream class for each section.

A stream that connects blocks from different sections keeps the stream class of the section where it originates.

For example, a flowsheet might have an upstream section that involves solids and a downstream section that does not (after all solids have been removed). You can assign stream class MIXCISLD to the upstream section and CONVEN to the downstream section.

You must use the Mixer and ClChng models to transition between flowsheet sections that are assigned different stream classes.

To assign a Stream Class to a flowsheet section:

1. From the Data menu, click Setup.
2. In the left pane of the Data Browser window, select the StreamClass form.
3. Click the Flowsheet sheet.
4. Use the list to select the name of the Stream Class associated with a given flowsheet section.

Specifying Stream Classes for Individual Streams

You can override the global or section stream class by specifying a stream class for one or more individual streams. To do this, use the StreamClass Streams sheet.

To assign streams to a Stream Class:

1. From the Data menu, click Setup.
2. In the left pane of the Data Browser window, click the StreamClass form.
3. Click the Streams sheet.

4. Select the streams to include in the stream class from the Available streams list and use the right arrow button to move them into the Selected streams list.

   Use the left arrow button to remove streams from the stream class. Use the double arrow button to move all of the streams in a list at one time.

   Streams that are left in the Available streams list will have the stream class for the flowsheet section (from the Flowsheet sheet).

Defining New Substreams

You need to define a new substream if:

- A simulation has more than one CISOLID or NC substream.
- You want to add a new PSD definition to a substream.

To create a new substream:

1. From the Data menu, click Setup.
2. In the left pane of the Data Browser, select the Substreams folder.
3. On the Substreams sheet, enter a new substream name in the Substream field.
4. In the Type field, select a substream type.

Use this type	For
MIXED	Conventional components that reach vapor-liquid-solid phase equilibrium
CISOLID (conventional inert solids)	Conventional components that appear in the solid phase but do not participate in phase equilibrium
NC (nonconventional)	Nonconventional components

5. If the substream type is CISOLID or NC, select a PSD in the Attribute field if desired.
6. Assign the substream to one or more stream classes. For more information, see Creating or Modifying Stream Classes on page 9-17.

About Particle Size Distributions

In Aspen Plus, particle size distribution is represented by the weight fractions per particle size interval, given the number of intervals and the size range for each interval.

The built-in Aspen Plus particle size distribution has 10 predefined size intervals. You can modify the built-in particle size distribution by changing the number of intervals or the size ranges for the intervals.

In some simulations you may want to have two or more particle size distribution definitions, with different size ranges. This is useful if different sections of your flowsheet have very different particle sizes.

For help on particle size distributions, click one of these topics:

- Specifying particle size distribution
- Changing particle size distribution intervals
- Creating new particle size distributions

Use the Setup Substreams form to create particle size distribution for a substream. You can specify the number of discrete intervals into which the particle size distribution is to be divided, and to specify the upper and lower size limits for each interval.

Changing Particle Size Distribution Intervals

To specify the number of intervals for the particle size distribution:

1. From the Data menu, click Setup.
2. In the left pane of the Data Browser window, select the Substreams folder.
3. In the Substreams Object Manager on the PSD sheet, select the name of the attribute set you want to modify and click Edit.
4. Type the number of intervals for the particle size distribution. You can also select the size units.
5. Type the limits for the particle size in all of the intervals.

   The Lower limit is automatically updated with the value of the Upper limit for the previous interval and vice versa.

Creating New Particle Size Distributions

You can create one or more new particle size distribution attributes, in addition to the built-in PSD:

1. From the Data menu, click Setup.
2. In the left pane of the Data Browser, select the Substreams folder.
3. In the Substreams Object Manager, on the PSD sheet, click New.
4. In the Create New ID dialog box, enter a PSD ID or accept the default ID.
5. On the PSD sheet, in the Interval Number column, enter the number of discrete intervals in the particle size distribution. You can also select the size units.
6. In the Lower Limit column, specify the lower size limit for each interval.

   Aspen Plus fills in the corresponding upper limit value automatically.
7. In the Upper Limit column, specify the upper size limit for the last interval.
8. You must assign the new PSD attribute to a substream class, on the Setup Substreams Substreams sheet.

For more information on defining a new substream, see Defining New Substreams on page 9-20 and Creating or Modifying Stream Classes on page 9-17.

Specifying Heat Streams

In Aspen Plus, material and energy balance reports consider only energy flows represented by streams. Any duty or power not represented by a heat or work stream appears on the report as an imbalance.

Any model that	Can have
Calculates heat duty	Outlet heat streams
Allows duty input specifications	Inlet heat streams

You can use an inlet heat stream to supply a heat duty specification to a unit operation block:

To display the Specifications sheet for the heat stream:

1. Double-click the stream in the flowsheet to select it.

   – or –

   From the Data menu, click Streams. In the Streams Object Manager, select the stream and click Edit.

2. On the Specifications sheet, specify the heat duty.

If the heat duty is	Then heat is
Positive	Supplied to the block
Negative	Removed from the block

3. In the destination block of the heat stream, leave the corresponding duty field blank. If you specify both an inlet heat stream and the heat duty in the destination block, the block specification is used.

Specifying Work Streams

In Aspen Plus, material and energy balance reports consider only energy flows represented by streams. Any duty or power not represented by a heat or work stream appears on the report as an imbalance.

Any model that	Can have
Allows power input specifications	Inlet work streams
Calculates power requirements	Outlet work streams

To use an inlet work stream to supply a power specification to a pump or compressor block:

1. Double-click the stream in the flowsheet to select it.

   – or –

   From the Data menu, click Streams. In the Streams Object Manager, select the stream and click Edit.

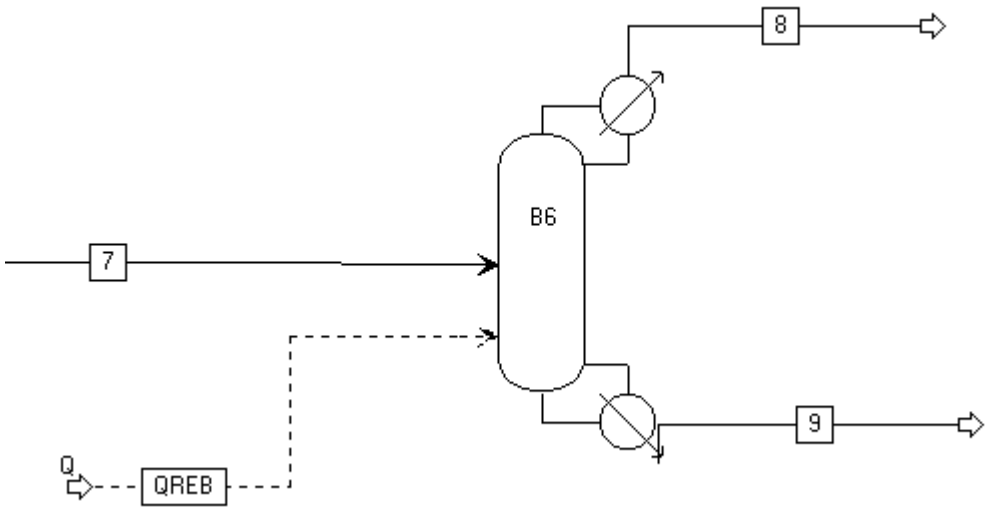
2. On the Specifications sheet, specify the power.

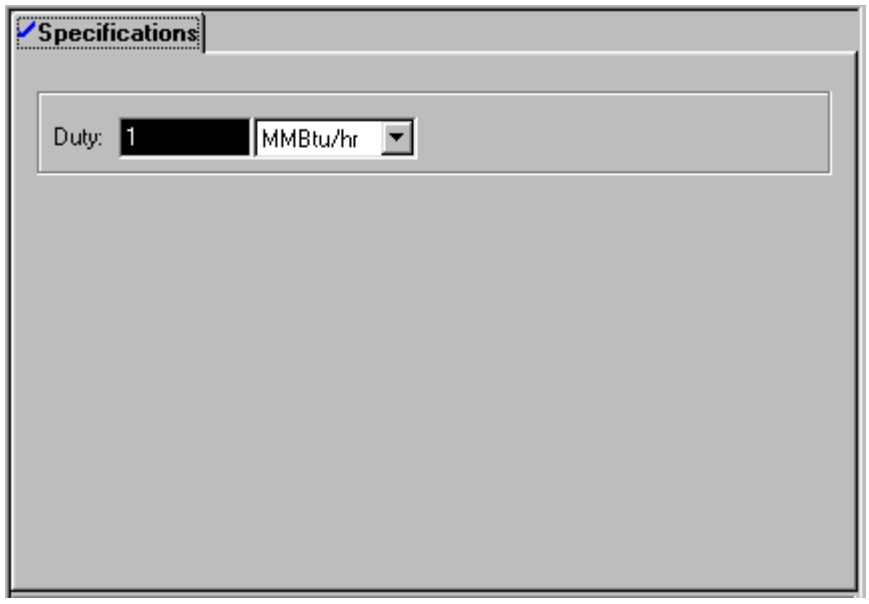
If the power is	Then work is
Negative	Supplied to a block
Positive	Removed from a block

3. In the destination block of the work stream, leave the corresponding power field blank. If you specify both an inlet work stream and the power in the destination block, the block specification is used.

Example of a Heat Stream to the Reboiler of a Column

Stream QREB supplies 1 MMBtu/hr of external heat duty to a RADFRAC block.





Using PseudoProduct Streams

You can define pseudoproduct streams to represent column internal flows, compositions, and thermodynamic conditions for these unit operations models:

- PetroFrac
- RadFrac
- MultiFrac
- RateFrac
- Extract
- CCD

You can use pseudoproduct streams to represent interconnecting streams in:

- PetroFrac
- MultiFrac
- RateFrac

The stream report includes pseudoproduct streams. Mass balance calculations for the block do not include the flow rates associated with pseudo-streams. The presence of pseudo-streams does not affect block results.

Pseudoproduct streams from one block may be an inlet to another block. Using a pseudo-stream as a block inlet results in an imbalance in the overall flowsheet material and energy balance report.

To define a pseudoproduct stream:

1. When creating the stream select a port labeled Pseudo Streams.
2. For each block that is connected to a pseudostream, complete the PseudoStream sheet(s) when specifying the block.

About Stream Libraries

Stream libraries store information about the composition and condition of material streams. If a stream is defined in a library, you can retrieve information from the library instead of entering data on the Streams forms. You must specify the stream library in the Run Settings dialog box before you run the simulation.

Use stream libraries to:

- Retrieve feed streams used frequently
- Transfer stream information from a previous simulation
- Initialize tear streams

A stream library can contain multiple cases. Each case usually represents the results of a previous simulation. When you retrieve results from a stream library, you specify the:

- Case(s) from which to retrieve results
- Streams in the current run that the stream library will fill in
- Substreams and components to be retrieved
- Component name translation, when the component IDs in the simulation are different from those in the library

For more information on creating stream libraries, see Chapter 35.

Accessing Stream Libraries

To specify that a run retrieves information about stream composition and conditions from a stream library:

1. From the Data menu, point to Flowsheeting Options, then Stream Library.
2. On the Specifications sheet, specify the case for the streams you want to retrieve.
3. If you are retrieving information for a single stream, enter the name of the stream from the library in the Stream Name in Library box.
4. If you specified the Stream Name in Library in Step 3, use the Include Stream option and enter the name of the stream in the current simulation. Otherwise select one of these options in the Streams field:

Option	To retrieve all streams with matching
All Streams	Stream ID
Include Streams	ID from a list you specify

5. In the Substreams and Components fields, specify the substreams and components you want to retrieve from the streams library.

   – or –

   Retrieve all substreams and components by leaving the fields blank.
6. In the State Variables field, specify the stream state variables that you want to retrieve from the stream library.
7. In the Component Mapping for Current Case section of the form, specify the mapping between the component ID in the current simulation and the component ID in the stream library. In the column on the left, enter the component ID from the current simulation. In the column on the right, enter the corresponding component IDs in the stream library.

– or –

On the Defaults sheet, define a default component mapping. Aspen Plus uses this mapping as the default for all cases.

8. Repeat Steps 2 through 8 for each case.

10 Unit Operation Models

The unit operation models are used to represent actual pieces of equipment, such as distillation columns or heat exchangers, commonly found in processing plants. To run a flowsheet simulation you must specify at least one unit operation model.

You choose unit operation models for flowsheet blocks when you define your simulation flowsheet (see Chapter 4).

Aspen Plus has a wide range of unit operation models to choose from. This chapter explains how to:

- Select the right unit operation model
- Enter model specifications
- Override global specifications at the block level
- Request heating/cooling curve calculations

Choosing the Right Unit Operation Model

This chapter provides a brief description of each model. For more detailed information, see the Aspen Plus reference manual *Unit Operation Models*.

Select appropriate unit operation models from the following table:

Unit Operation Models

Type	Model	Description
Mixers/Splitters	Mixer	Stream mixer
	FSplit	Stream splitter
	SSplit	Substream splitter
Separators	Flash2	Two-outlet flash
	Flash3	Three-outlet flash
	Decanter	Liquid-liquid decanter
	Sep	Multi outlet component separator
	Sep2	Two-outlet component separator
Heat Exchangers	Heater	Heater/cooler
	HeatX	Two-stream heat exchanger
	MheatX	Multistream heat exchanger
	HxFlux	Interface to BJAC Shell & Tube heat exchanger program
	Hetran †	Interface to BJAC air cooled heat exchanger program
	Aerotran †	Interface to the Aspen Aerotran program
	HTRIIST	Interface to the IST program
Columns	DSTWU	Shortcut distillation design
	Distl	Shortcut distillation rating
	RadFrac	Rigorous distillation
	Extract	Rigorous liquid-liquid extractor
	MultiFrac	Rigorous distillation for complex columns
	SCFrac	Shortcut distillation for petroleum
	PetroFrac	Rigorous distillation for petroleum
	RateFrac †	Rate-based distillation
	BatchFrac †	Rigorous batch distillation
Reactors	RStoic	Stoichiometric reactor
	RYield	Yield reactor
	REquil	Equilibrium reactor
	RGibbs	Equilibrium reactor
	RCSTR	Continuous-stirred tank reactor
	RPlug	Plug flow reactor
	RBatch	Batch reactor
Pressure Changers	Pump	Pump/hydraulic turbine
	Compr	Compressor/turbine
	MCompr	Multistage compressor/turbine
	Pipeline	Multi segment pipeline pressure drop
	Pipe	Single segment pipeline pressure drop
	Valve	Rigorous valve pressure drop

Continued

Unit Operation Models (continued)

Type	Model	Description
Manipulators	Mult	Stream multiplier
	Dupl	Stream duplicator
	ClChng	Stream class changer
Solids	Crystallizer	Mixed suspension mixed product removal crystallizer
	Crusher	Solids crusher
	Screen	Solids separator
	FabFl	Fabric filter
	Cyclone	Cyclone separator
	VScrub	Venturi scrubber
	ESP	Electrostatic precipitator
	HyCyc	Hydrocyclone
	CFuge	Centrifuge filter
	Filter	Rotary vacuum filter
	SWash	Single-stage solids washer
	CCD	Counter-current decanter
User models	User	User-supplied unit operation model
	User2	User-supplied unit operation model

† *RateFrac, BatchFrac, Hetran, and Aerotran require a separate license and can be used only by customers who have purchased the right to use them through specific license agreements with Aspen Technology, Inc.*

Mixers and Splitters

This section describes the models that can be used to mix or split flowsheet streams.

The Mixer unit operation model combines streams. FSplit and SSplit combine feed streams and then split the resulting stream, based on your specifications.

Mixer

Mixer combines material streams (or heat streams or work streams) into one outlet stream. If material streams are mixed, you can use an optional water decant stream to decant free water from the outlet. You can specify an outlet pressure or pressure drop for material streams. The mixer model determines the combined outlet stream temperature and phase condition by performing an adiabatic phase equilibrium flash calculation on the composite feed streams.

Mixer can be used to model mixing tees, or other types of stream mixing operations.

FSplit

FSplit combines material streams (or heat streams or work streams) and divides the resulting stream into two or more outlet streams. All outlets have the same composition and properties.

Use FSplit to model flow splitters and purges or vents. You must provide specifications for all but one outlet stream. FSplit calculates the flowrate of the unspecified stream.

SSplit

SSplit combines material streams and divides the resulting stream into two or more outlet streams. SSplit allows specification of streams with various substreams.

You must specify the splits of each substream, for all but one outlet stream. SSplit calculates the flowrate of each substream in the unspecified outlet stream. For more information about substreams, see Chapter 9.

For example, you can use SSplit to perfectly separate a stream containing both liquid and solid phases into two streams each containing only one pure phase. You can also use SSplit to model other solid stream splitters, bleed valves, purges or vents.

Separators

The Separator Blocks, Sep and Sep2, combine feed streams and then split the resulting stream, based on your specifications. When the details of the separation are unknown or unimportant, you can use Sep and Sep2 instead of rigorous separation models (such as distillation or absorption models) to save computational time.

The flash models, Flash2 and Flash3, determine the thermal and phase conditions of a mixture with one or more inlet streams. You can generate heating or cooling curve tables for these models.

The flash models represent single stage separators such as knock-out drums. They perform a phase equilibrium flash calculation based on your specifications. Adiabatic, isothermal and isobaric flashes, and dew or bubble points, are among the calculations these models perform.

In general, to fix the thermodynamic condition of inlet streams, you must specify a combination of any two of:

- Temperature
- Pressure
- Heat duty
- Molar vapor fraction

This table shows you what to set the molar vapor fraction as:

To Determine	Set the Molar Vapor Fraction
The dew point of a mixture	1
The bubble point of a mixture	0

The combination of heat duty and molar vapor fraction is not allowed in the flash models.

Flash2

Flash2 performs rigorous 2 (vapor-liquid) or 3 (vapor-liquid-liquid) phase equilibrium calculations. Flash2 produces one vapor outlet stream, one liquid outlet stream, and an optional water decant stream.

You can use Flash2 to model flashes, evaporators, knock-out drums, and any other single-stage separators, with sufficient vapor disengagement space. Optionally, you can specify a percentage of the liquid phase to be entrained in the vapor stream.

Flash3

Flash3 performs rigorous 3 phase vapor-liquid-liquid equilibrium calculations, to produce one vapor outlet stream and two liquid outlet streams.

You can use Flash3 to model any single-stage separator with sufficient vapor-liquid disengagement space as well as two liquid phase settling space. You can specify entrainment of each liquid phase in the vapor stream.

The vapor outlet stream can have a flow rate of zero for a decanter with no vapor-liquid disengagement. If you do not know whether there is a vapor phase, use the Flash3 model instead of the Decanter model.

Decanter

Decanter models knock-out drums, decanters, and other single-stage separators with sufficient residence time for separation of two liquid phases but without a vapor phase.

Decanter determines the thermal and phase conditions of a mixture with one or more inlet streams, at the specified temperature or heat duty.

Decanter can calculate liquid-liquid distribution coefficients from:

- Physical property method
- User supplied distribution correlation
- User supplied Fortran subroutine

For information about writing Fortran subroutines, see *Aspen Plus User Models*.

Since the Decanter model assumes implicitly that there is no vapor phase formation, use Flash3 if you suspect any vapor phase formation.

Sep

Sep combines inlet streams and separates the resulting stream into two or more streams, according to splits you specify for each component. You can specify the splits for each component in each substream.

You can use the Sep model to represent component separation operations such as a distillation column when fractionation achieved or desired by the column is known but the details of the column energy balance are unknown or unimportant.

Sep2

Sep2 combines inlet streams and separates the resulting stream into two outlet streams. Sep2 is similar to Sep, but offers a wider variety of specifications, such as component purity or recovery. These specifications make it even easier to represent component separation operations such as a distillation column when fractionation achieved or desired by the column is known but the details of the separation are unknown or unimportant.

Heat Exchangers

All heat exchangers determine the thermal and phase conditions of a mixture with one or more inlet streams. The heat exchanger models simulate the performance of heaters or two or multi stream heat exchangers. You can generate heating or cooling curve tables for all models described in this section.

Heater

Heater performs these types of single phase or multiphase calculations:

- Bubble or dew point calculations
- Add or remove any amount of user specified heat duty
- Match degrees of superheating or subcooling
- Determine heating or cooling duty required to achieve a certain vapor fraction

Heater produces one outlet stream, with an optional water decant stream. The heat duty specification may be provided by a heat stream from another block.

You can use Heater to model:

- Heaters or coolers (one side of a heat exchanger)
- Valves when you know the pressure drop
- Pumps and compressors whenever you do not need work-related results

You can also use Heater to set or change the thermodynamic condition of a stream.

HeatX

HeatX can perform shortcut or detailed rating calculations for most types of two-stream heat exchangers. The main difference between the two calculation methods is the procedure for the calculation of the overall heat transfer coefficient.

The shortcut method always uses a user specified (or default) value for the overall heat transfer coefficient.

The detailed method uses rigorous heat transfer correlations for film coefficients and combines the resistances due to shell and tube side films with the wall resistance to calculate the overall heat transfer coefficient. You need to know the geometry to use the detailed method.

You must specify the hot and cold inlet streams and one of these performance specifications for your heat exchanger:

- Outlet temperature or temperature change of the hot or cold stream
- Molar vapor fraction of the hot or cold stream
- Degree of superheating (subcooling) of cold (hot) stream
- Heat exchanger duty
- Surface heat transfer area
- Temperature approach at the hot or cold stream outlet

Shortcut Method for HeatX

For the shortcut method you may specify a pressure drop for each side of the heat exchanger. The HeatX model determines the outlet stream conditions based on heat and material balances and uses a constant value for the heat transfer coefficient to estimate the surface area requirement. You may also provide phase specific heat transfer coefficients.

Detailed Method for HeatX

HeatX can also perform detailed rating calculations by modeling a wide variety of shell and tube heat exchanger types rigorously, including:

- Countercurrent and co-current
- Segmental baffle TEMA E, F, G, H, J, and X shells
- Rod baffle TEMA E and F shells
- Bare and low-finned tubes

HeatX can perform a full zone analysis with heat transfer and pressure drop estimation for single and two-phase streams. For rigorous heat transfer and pressure drop calculations, you must supply the exchanger geometry.

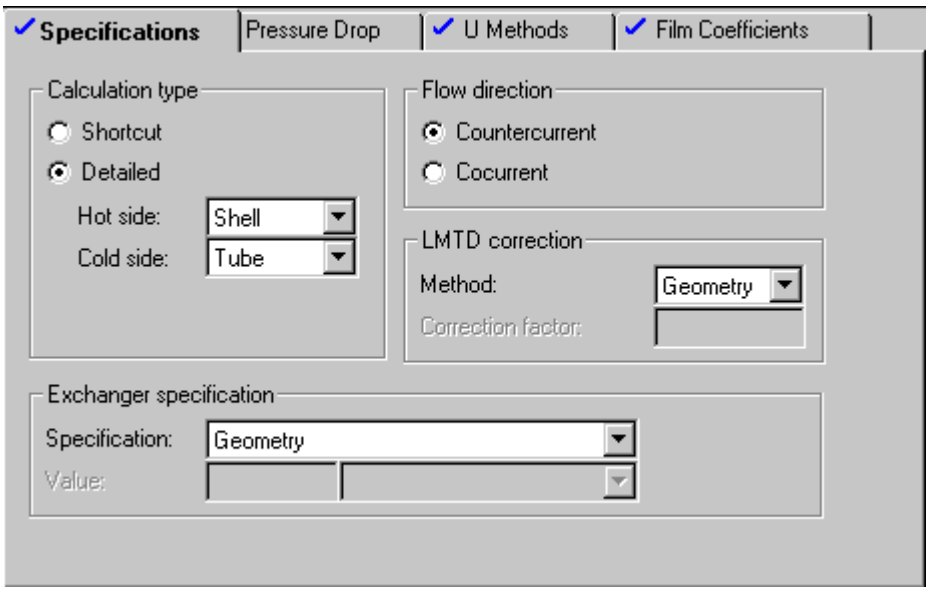
HeatX has correlations to estimate sensible heat, nucleate boiling, and condensation film coefficients.

HeatX cannot:

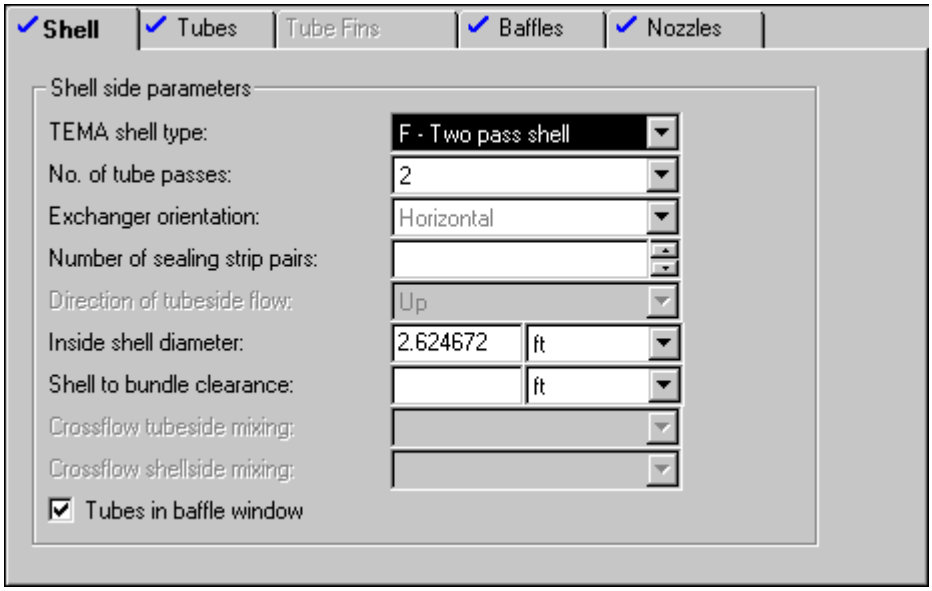
- Perform design calculations (use Hetran or Aerotran)
- Perform mechanical vibration analysis
- Estimate fouling factors

Example of Specification for a Shell and Tube Heat Exchanger

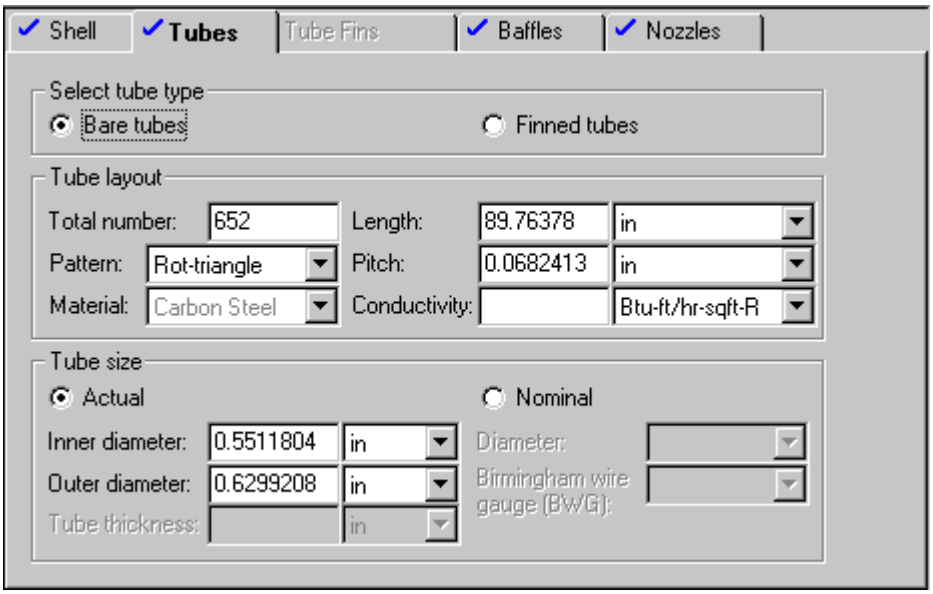
Use the detailed calculation type to rate the performance of countercurrent shell and tube heat exchanger, where the hot fluid is on the shell side.



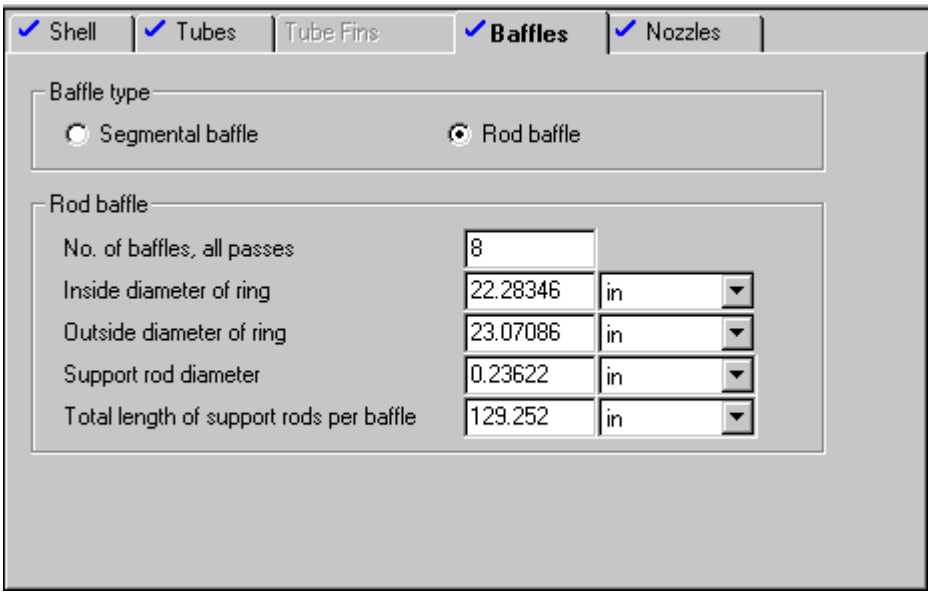
Specify the shell TEMA type, diameter, and orientation.



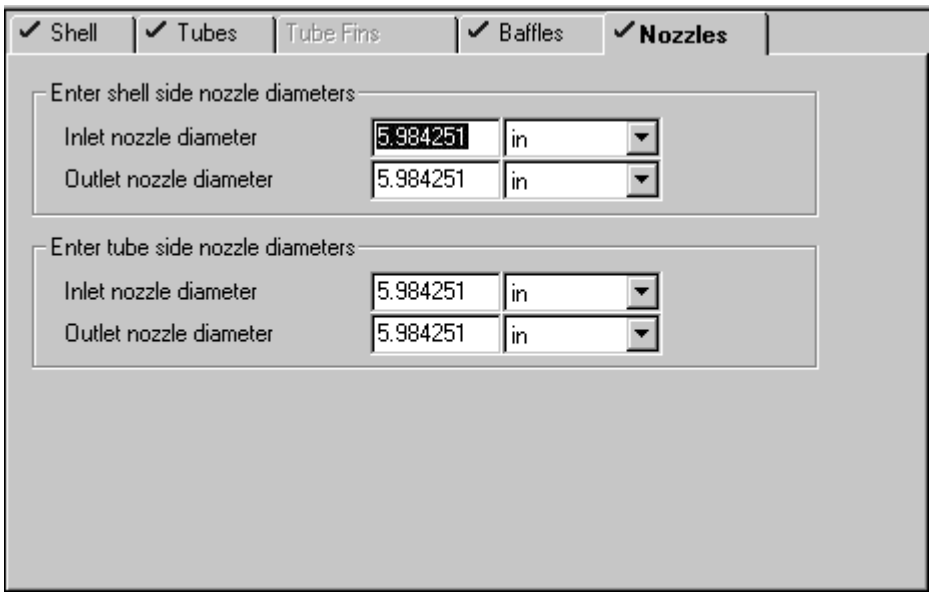
Specify tube side data.



Specify baffle type, spacing and dimensions:



Specify the shell and tube side nozzle diameters:



MHeatX

MHeatX represents heat transfer between multiple hot and cold streams, as in an LNG exchanger. It can also model two-stream heat exchangers. You can decant free water from any outlet stream. An MHeatX block is divided into multiple heaters connected by heat streams. This configuration usually leads to faster flowsheet convergence.

MHeatX does not use or calculate heat transfer coefficients, but it can calculate the overall UA for the exchanger and perform a detailed zone analysis.

HxFlux

HxFlux is used to perform heat transfer calculations between a heat sink and a heat source, using convective heat transfer. The driving force for the convective heat transfer is calculated as a function of log-mean temperature difference or LMTD.

You can specify variables among the inlet and outlet stream temperatures, duty, heat transfer coefficient, and heat transfer area. HxFlux calculates the unknown variable and determines the log mean temperature differences, using either the rigorous or the approximate method.

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Hetran

Hetran is the interface to the Aspen Hetran program for designing and simulating shell and tube heat exchangers. Use Hetran to simulate shell and tube heat exchangers with a wide variety of configurations.

To use Hetran:

1. Place the block in the flowsheet.
2. Connect inlet and outlet streams.
3. Specify the name of the B-JAC input file for that exchanger and a few optional parameters.

Information related to the heat exchanger configuration and geometry are entered through the Hetran program interface. The exchanger specification is then saved in the Hetran input file format.

You do not have to enter information about the exchanger's physical characteristics for the blocks or through input language. That information is retrieved from the B-JAC input file that you specify.

Aerotran

Aerotran is the interface to the Aspen Aerotran program for designing and simulating air-cooled heat exchangers.

Aerotran can be used to simulate air-cooled heat exchangers with a wide variety of configurations. It can also be used to model economizers and the convection section of fired heaters.

To use Aerotran:

1. Place the block in the flowsheet.
2. Connect the inlet and outlet streams.
3. Specify the name of the B-JAC input file for that exchanger and a few optional parameters.

Information related to the air cooler configuration and geometry are entered through the Aerotran program interface. The air cooler specification is saved in the Aerotran input file format. You do not have to enter information about the air cooler's physical characteristics. That information is retrieved from the B-JAC input file that you specify.

HTRIIST

HTRIIST is the interface to the IST program from the Heat Transfer Research Institute (HTRI) for designing and simulating shell and tube heat exchangers. Use HTRIIST to simulate shell and tube heat exchangers with a wide variety of configurations.

To use HTRIIST:

1. Place the block in the flowsheet.
2. Connect inlet and outlet streams.
3. Specify the name of the IST input file for that exchanger and a few optional parameters.

Information related to the heat exchanger configuration and geometry are entered through the IST program interface. The exchanger specification is then saved in the IST input file format.

You do not have to enter information about the exchanger's physical characteristics for the blocks or through input language. That information is retrieved from the IST input file that you specify.

Columns

The models for shortcut distillation are DSTWU, Distl, and SCFrac.

DSTWU and Distl:

- Are for single columns
- Can perform free-water calculations in the condenser
- Allow you to use water decant streams to decant free water from the condenser

SCFrac performs shortcut distillation calculations for petroleum refining units, such as crude units and vacuum towers.

Aspen Plus provides four rigorous multistage separation models:

Model	Purpose
RadFrac	General vapor-liquid multistage separation
MultiFrac	General systems of interlinked multistage distillation units
PetroFrac	Petroleum refining fractionation units
RateFrac	Rate-based non-equilibrium separation

Extract is a rigorous model for simulating liquid-liquid extractors. It is appropriate only for rating calculations.

DSTWU

DSTWU performs a Winn-Underwood-Gilliland shortcut design calculation for a single-feed, two-product distillation column, with a partial or total condenser. For the specified recovery of the light and heavy key components, DSTWU estimates the minimum for either:

- Reflux ratio
- Number of theoretical stages

DSTWU estimates one of the following requirements:

- Reflux ratio given the number of theoretical stages
- Number of theoretical stages given the reflux ratio

DSTWU also estimates:

- Optimum feed stage location
- Condenser and reboiler duties

DSTWU can produce tables and plots of reflux ratio versus number of stages.

Distl

Distl is a shortcut multicomponent distillation rating model. This model uses the Edmister approach to separate an inlet stream into two products. You must specify:

- Number of theoretical stages
- Reflux ratio
- Overhead product rate

Distl estimates the condenser and reboiler duties. You can specify a partial or a total condenser.

SCFrac

SCFrac models petroleum refining towers, such as crude units and vacuum towers. SCFrac performs shortcut distillation calculations for columns with a single feed, one optional stripping steam stream, and any number of products.

SCFrac models an n-product refining tower with n–1 sections.

Based on your product specifications and fractionation indices, SCFrac estimates:

- Product composition and flows
- Number of stages per section
- Heating or cooling duty for each section

SCFrac does not handle solids.

RadFrac

RadFrac is a rigorous model for simulating all types of multistage vapor-liquid fractionation operations. In addition to ordinary distillation, it can simulate:

- Absorption
- Reboiled absorption
- Stripping
- Reboiled stripping
- Extractive and azeotropic distillation

RadFrac is suitable for:

- Three-phase systems
- Narrow-boiling and wide-boiling systems
- Systems exhibiting strong liquid phase nonideality

RadFrac can detect and handle a free-water phase or other second liquid phase anywhere in the column. You can decant free water from the condenser.

RadFrac can handle solids on every stage.

RadFrac can model columns where chemical reactions are occurring. Reactions can have fixed conversions, or they can be:

- Equilibrium
- Rate-controlled
- Electrolytic

RadFrac can model columns where two liquid phases exist and different chemical reactions occur in the two liquid phases. RadFrac can also model salt precipitation.

RadFrac can operate in rating mode or design mode.

Rating Mode

In rating mode RadFrac calculates:

- Temperature
- Flow rate
- Mole fraction profiles

These profiles are based on specified column parameters, such as reflux ratio, product rates, and heat duties.

All rating mode flow specifications can be in mole, mass, or standard liquid volume units.

You can specify component or stage efficiencies.

RadFrac accepts both Murphree and vaporization efficiencies. You can manipulate Murphree efficiencies to match plant performance.

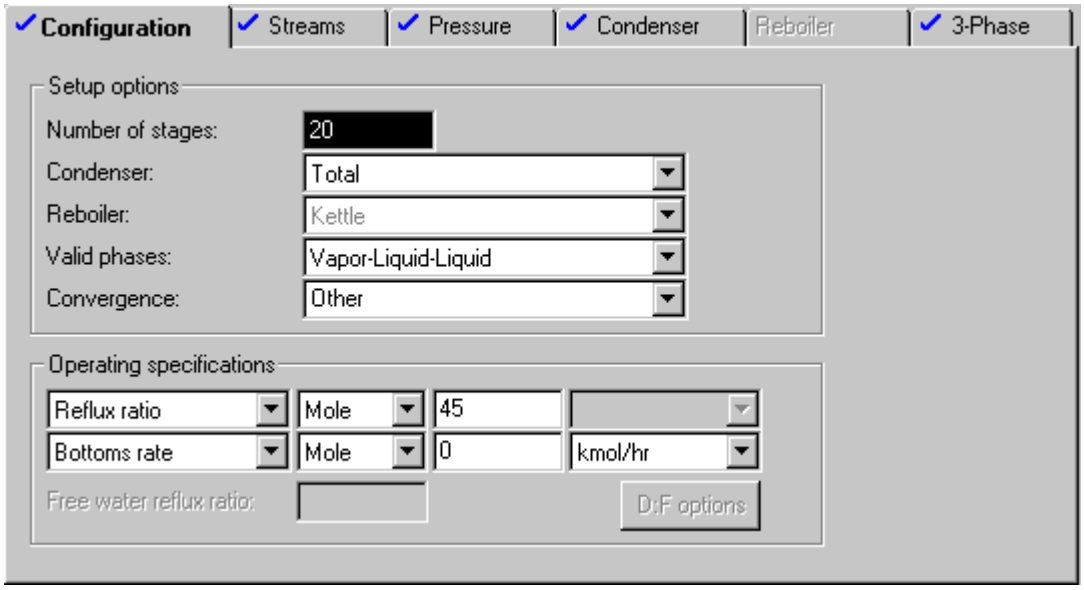
Design Mode

In design mode, you can specify temperatures, flow rates, purities, recoveries, or stream properties anywhere in the column. Examples of stream properties are volume flow and viscosity. You can specify all flow, flow ratio, composition, and recovery specifications in mole, mass, or standard liquid volume units.

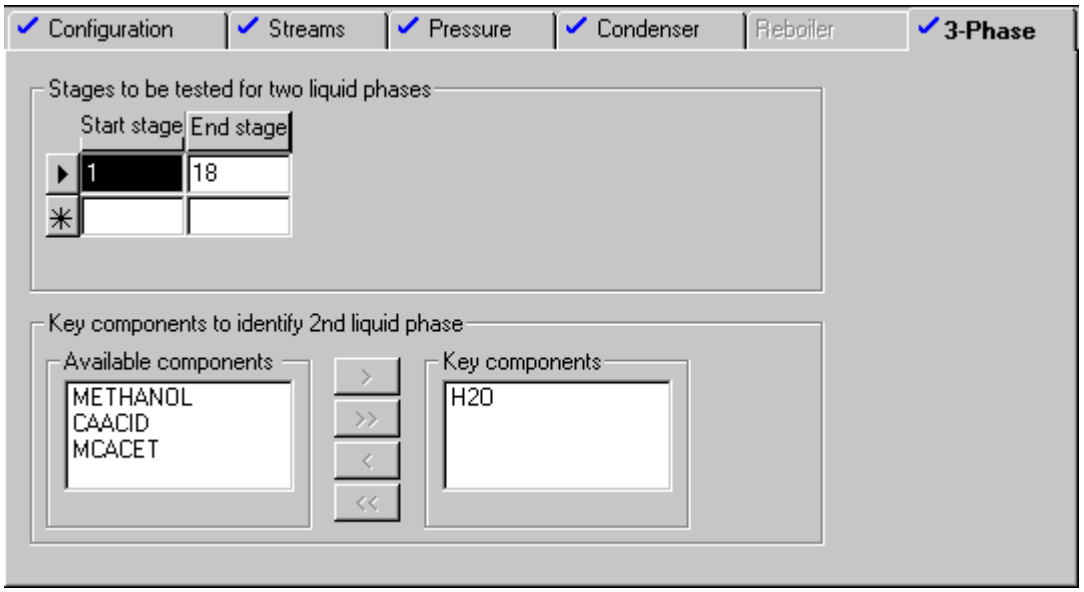
RadFrac has extensive capabilities for sizing and rating trays and packings. You can choose from several common tray types, and random and structured packings.

Example of Specifying a Reactive 3-phase Distillation Column

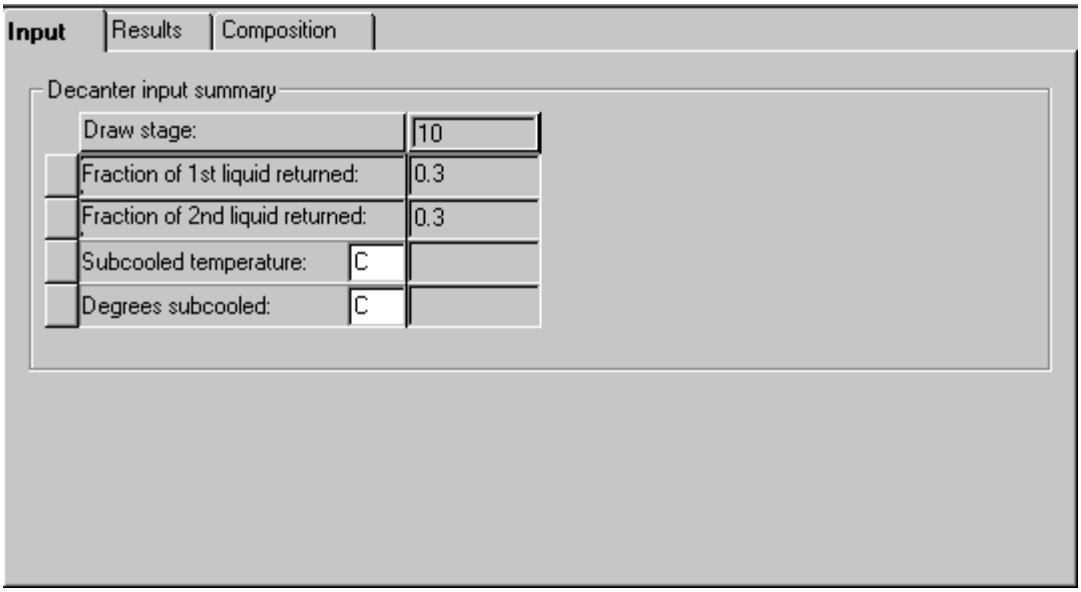
The following example shows the specifications for a reactive 3-phase distillation column without a bottoms product and a reflux ratio of 45. The column has 18 equilibrium stages and a total condenser and a kettle reboiler.



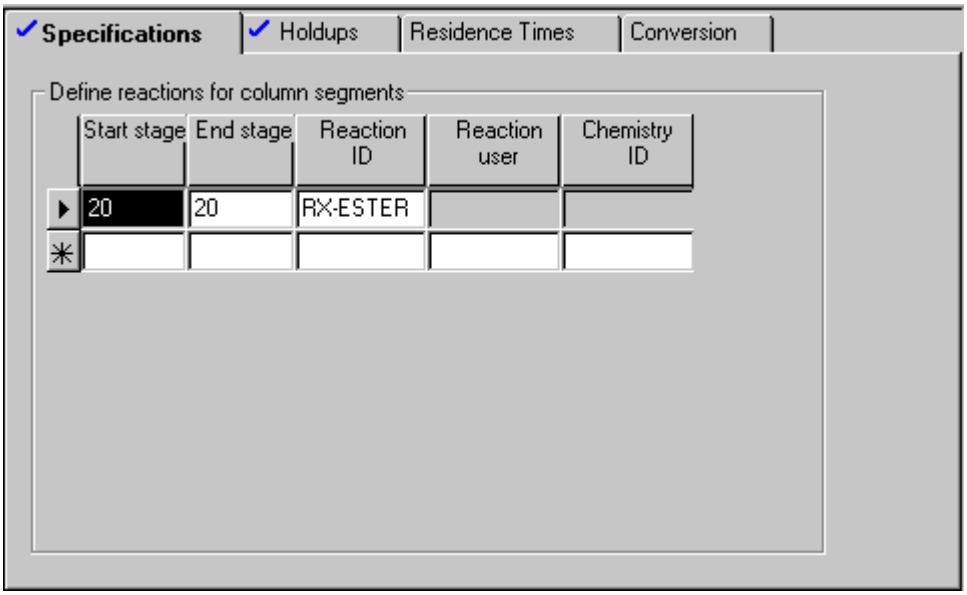
All stages from the condenser (stage 1) through stage 18 are checked for presence of an aqueous second liquid phase.



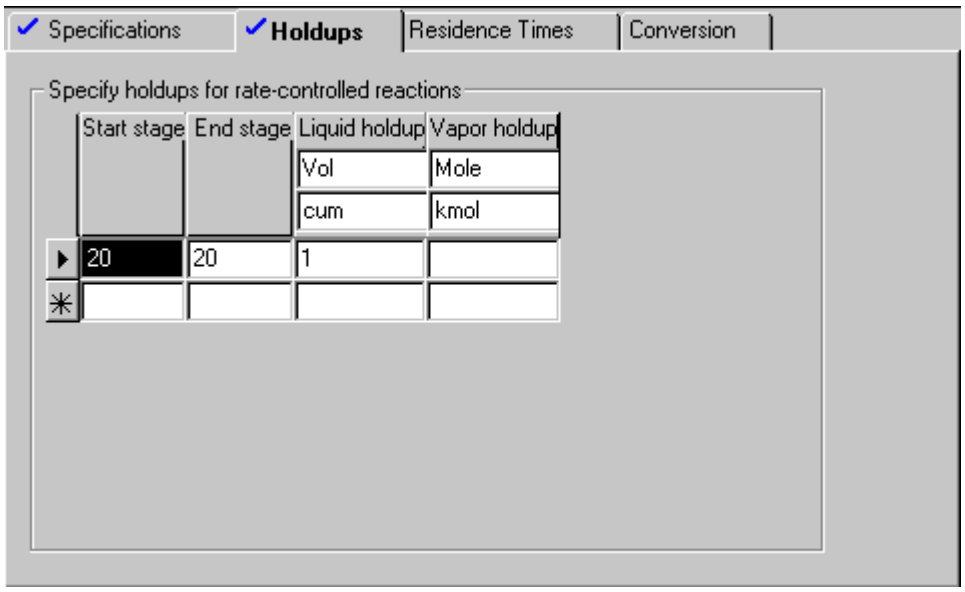
A liquid decanter is specified on equilibrium stage 10 which returns 30% of total liquid flow.



The reactions occur only in the reboiler. The reaction rate and stoichiometry are referenced from a Reaction ID defined in the Reactions folder.



The total liquid holdup (reaction volume) is 1 m^3.



MultiFrac

MultiFrac is a rigorous model for simulating general systems of interlinked multistage fractionation units. MultiFrac models a complex configuration consisting of:

- Any number of columns, each with any number of stages
- Any number of connections between columns or within columns
- Arbitrary flow splitting and mixing of connecting streams

MultiFrac can handle operations with:

- Side strippers
- Pumparounds
- Bypasses
- External heat exchangers
- Single-stage flashes
- Feed furnaces

Typical MultiFrac applications include:

- Heat-integrated columns, such as Petlyuk towers
- Air separation column systems
- Absorber/stripper combinations
- Ethylene plant primary fractionators

You can also use MultiFrac for petroleum refining fractionation units, such as atmospheric crude units and vacuum units. But for these applications PetroFrac is more convenient to use. Use MultiFrac only when the configuration is beyond the capabilities of PetroFrac.

MultiFrac can detect a free-water phase in the condenser or anywhere in the column. It can decant the free-water phase on any stage.

Although MultiFrac assumes equilibrium stage calculations, you can specify either Murphree or vaporization efficiencies. You can use MultiFrac for sizing and rating trays and packings. MultiFrac can model both random and structured packings.

PetroFrac

PetroFrac is a rigorous model designed for simulating complex vapor-liquid fractionation operations in the petroleum refining industry. Typical operations include:

- Preflash tower
- Atmospheric crude unit
- Vacuum unit
- FCC main fractionator
- Delayed coker main fractionator
- Vacuum lube fractionator

You can also use PetroFrac to model the primary fractionator in the quench section of an ethylene plant.

PetroFrac can model the feed furnace together with the fractionation towers and strippers in an integrated fashion. With this feature, you can easily analyze the effect of furnace operating parameters on tower performance.

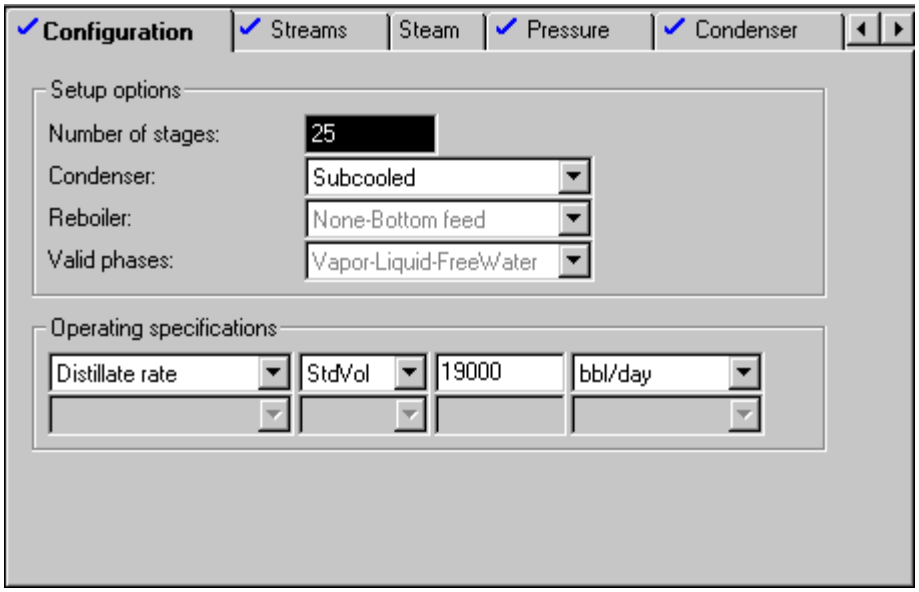
PetroFrac can detect a free-water phase in the condenser or anywhere in the column. It can decant the free-water phase on any stage.

Although PetroFrac assumes equilibrium stage calculations, you can specify either Murphree or vaporization efficiencies.

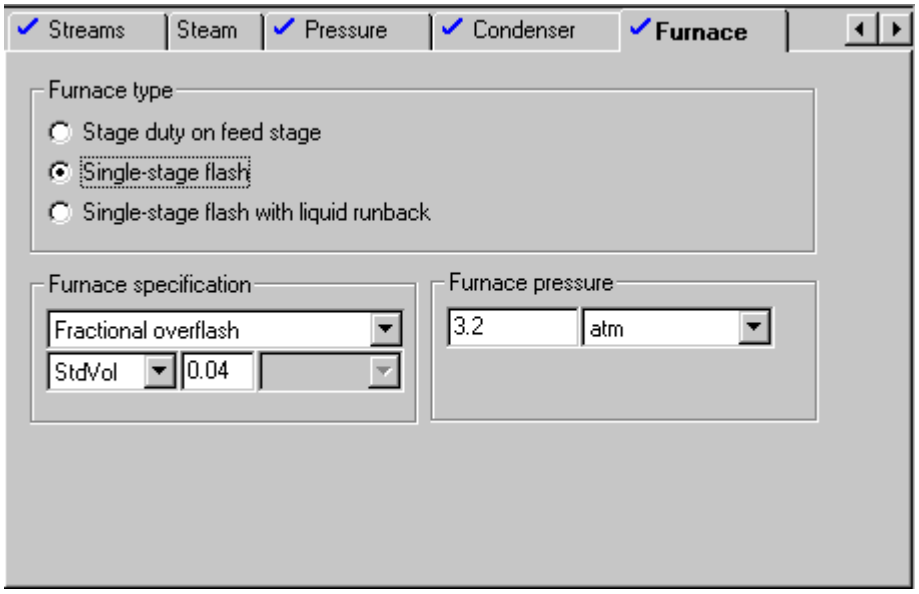
You can use PetroFrac to size and rate columns consisting of trays and/or packings. PetroFrac can model both random and structured packings.

Example of Specifying an Atmospheric Crude Oil Tower

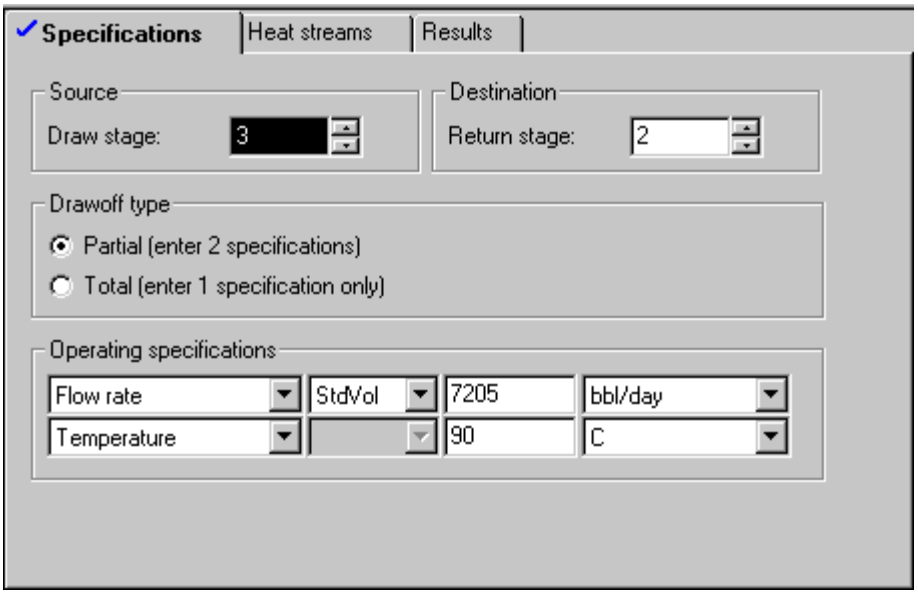
This example illustrates the specifications for an atmospheric crude oil tower consisting of 25 equilibrium stages (including a total condenser) in the main column, 2 pumparounds, and three side strippers. The top distillate rate is set at 19,000 BPD.



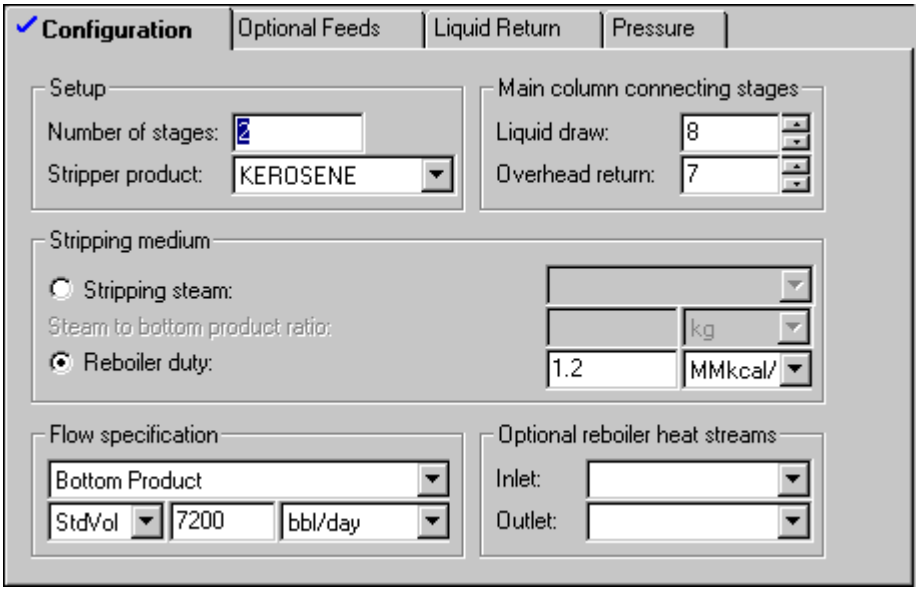
The column feed passes through a furnace which operates at 3.2 atm and the overflash stream is specified to be 4% of the column feed by volume.



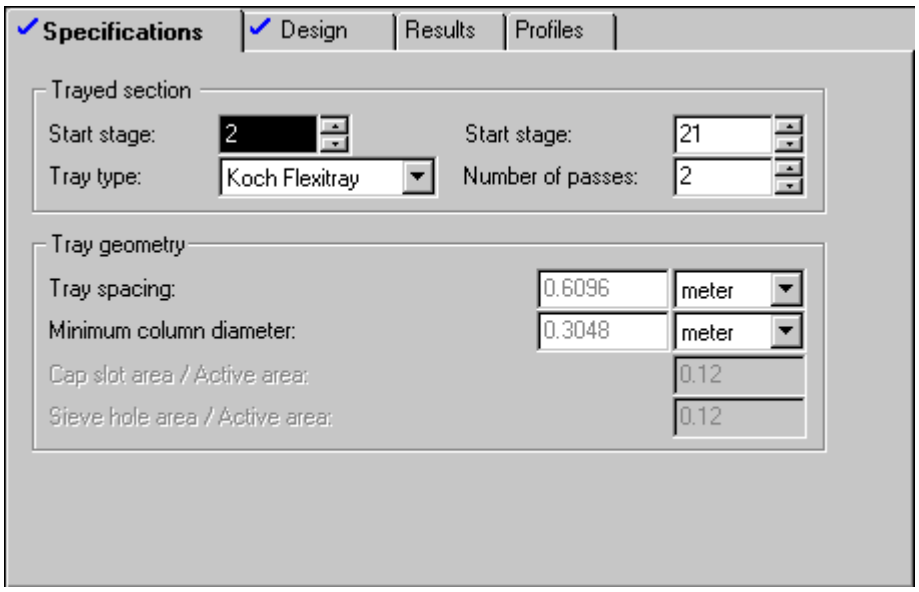
The first pumparound rate is 7,205 BPD and is a partial stream drawn from stage 3 and is returned to stage 2 at 90 C.



The first sidestripper has 2 equilibrium stages and strips light ends from the 7,200 BPD of Kerosene product stream which is drawn from stage of the main column. The stripped vapors are returned to main column on stage 8. The reboiler duty is 1.2 MMkcal/hr.



The main column is to be sized based on 2-pass Koch Flexitray trays on stages 2 through 21.



RateFrac

RateFrac is a rate-based model for non-equilibrium separation. It simulates actual tray and packed columns, rather than idealized representations.

RateFrac:

- Explicitly accounts for the interphase mass and heat transfer processes.
- Simulates single and interlinked columns involving vapor-liquid fractionation operations such as absorption, distillation, and stripping.

Use RateFrac for

- Systems with both a vapor and a liquid phase. RateFrac can detect a free-water phase only in the condenser.
- Nonreactive systems
- Reactive systems
- Electrolyte systems

RateFrac does not use empirical factors, such as efficiencies and the Height Equivalent of a Theoretical Plate (HETP). RateFrac treats separation as a mass and heat transfer rate process, instead of an equilibrium process. The degree of separation achieved between the contacting phases depends on the extent of mass and heat transfer between phases. The transfer rates between phases are strongly affected by the extent to which the phases are not in equilibrium. RateFrac assumes that thermodynamic equilibrium prevails only at the vapor-liquid interface separating the contacting phases.

Batch Distillation - BatchFrac

BatchFrac is the unit operation model for batch distillation. It is a a rigorous model for simulating multistage batch distillation columns.

BatchFrac uses a robust and efficient algorithm to solve the unsteady-state heat and material balance equations that describe the behavior of batch distillation processes. Rigorous heat balances, material balances, and phase equilibrium relationships are applied at each stage.

BatchFrac can handle a wide variety of batch distillation problems, including these systems:

- Narrow-boiling
- Wide-boiling
- Highly non-ideal
- Three-phase
- Reactive

BatchFrac can detect the presence of a free-water phase in the condenser, or of any second liquid phase anywhere in the column. BatchFrac has complete flexibility in handling interstage decanters.

Use BatchFrac to simulate batch distillation columns with equilibrium-controlled reactions or rate-controlled reactions. These reactions can occur on any stage, including the reboiler and condenser.

BatchFrac assumes:

- Equilibrium stages are used. (However, you can specify vaporization efficiencies.)
- There is constant liquid holdup and no vapor holdup.
- Column hydraulics are not modeled.

Extract

Extract is a rigorous model for simulating liquid-liquid extractors. It is appropriate only for rating calculations.

Extract can have multiple feeds, heater/coolers, and sidestreams. To calculate distribution coefficients, use one of the following:

- An activity coefficient model
- An equation of state capable of representing two liquid phases
- A built-in temperature-dependent polynomial
- A Fortran subroutine

Extract accepts specifications for component or stage efficiencies.

Reactors

Chemical reactions occur under diverse conditions in many different types of equipment.

Aspen Plus provides seven models for chemical reactor simulations:

Model	Purpose
RStoic	Conversion reactor with known stoichiometry
RYield	Yield reactor with known product yields
REquil	Two-phase chemical equilibrium reactor (stoichiometric)
RGibbs	Multiphase chemical equilibrium reactor (non-stoichiometric)
RCSTR	Continuous stirred tank reactor with known kinetics
RPlug	Plug flow reactor with known kinetics
RBatch	Batch or semi-batch reactor with known kinetics

RStoic, RYield, RGibbs, and RCSTR can have any number of material feed streams, which are mixed internally. Heats of reaction are not required for any reactor model. Aspen Plus calculates heats of reaction using heats of formation.

For RCSTR, RPlug, and RBatch, you must provide reaction kinetics information using:

- The built-in power law model
- The built-in generalized Langmuir-Hinschelwood-Hougen-Watson (LHHW) model
- A user-written Fortran subroutine (For more information, see *Aspen Plus User Models*)

RStoic

RStoic models a reactor when:

- Reaction kinetics are unknown or unimportant.
- Stoichiometry is known.
- You can specify the extent of reaction or conversion.

Rstoic can handle reactions that occur independently in a series of reactors. It can also perform product selectivity and heat of reaction calculations.

RYield

RYield models a reactor by specifying reaction yields of each component. This model is useful when:

- Reaction stoichiometry and kinetics are unknown.
- Yield distribution data or correlations are available.

REquil

REquil models reactors when some or all reactions reach equilibrium. REquil can calculate single-phase chemical equilibrium, or simultaneous phase and chemical equilibria. REquil calculates equilibrium by solving stoichiometric chemical and phase equilibrium equations.

RGibbs

RGibbs models single-phase chemical equilibrium, or simultaneous phase and chemical equilibria. You must specify the reactor temperature and pressure, or pressure and enthalpy. RGibbs minimizes Gibbs free energy, subject to atom balance constraints. This model does not require reaction stoichiometry. RGibbs can determine phase equilibrium without chemical reaction, particularly for multiple liquid phases. Any number of liquid phases are allowed.

You can model solids in RGibbs either as single condensed species and/or as solid solution phases.

You can also assign components to be in particular phases in equilibrium. You can use different property models for each liquid or solid solution phase. This capability makes RGibbs particularly useful for:

- Pyrometallurgical applications
- Modeling ceramics and alloys

RGibbs accepts restricted equilibria specifications. You can restrict equilibrium by specifying:

- Fixed moles of any product
- Percentage of a feed component that does not react
- Temperature approach to equilibrium for the entire system
- Temperature approaches for individual reactions
- Fixed extents of reaction

RCSTR

RCSTR rigorously models a continuous-stirred tank reactor. You can use this model when:

- Reaction kinetics are known.
- The contents of the reactor have the same properties as the outlet stream.

RCSTR can model equilibrium reactions simultaneously with rate-based reactions.

RCSTR computes one of the following for the reactor:

- Heat duty given the temperature
- Temperature given the heat duty

RPlug

RPlug rigorously models plug flow reactors. A cooling stream around the reactor is optional. You can also use RPlug to model reactors with cocurrent and countercurrent coolant streams. RPlug handles rate-based kinetic reactions only.

RBatch

RBatch rigorously models batch or semi-batch reactors. Holding tanks are used to interface the batch reactor with the steady-state streams of an Aspen Plus simulation.

For semi-batch reactors, you can specify a continuous vent and any number of continuous or delayed feeds. RBatch handles rate-based kinetic reactions only.

Pressure Changers

Pump and compressor models change pressures when energy-related information, such as power requirement, is needed or known. Free water can be decanted from the Pump or Compr products, or from the MCompr intercoolers. For pressure changes only use other models, such as Heater or Valve.

Pipeline calculates the pressure drop and heat transfer in a pipe segment or a pipeline. Pipeline can model any number of segments to describe the pipe geometry.

Pipe calculates the pressure drop and heat transfer for a single pipe segment with fittings.

Valve rigorously models the pressure drop in control valves.

Pump

Pump simulates a pump or hydraulic turbine. This model calculates either the power requirement or the power produced, given an outlet pressure specification. Pump can calculate the outlet pressure, given a power specification.

Compr

Compr simulates a:

- Polytropic compressor
- Polytropic positive displacement compressor
- Isentropic compressor
- Isentropic turbine

Compr calculates either the power requirement given an outlet pressure specification, or the outlet pressure given a power specification.

MCompr

MCompr simulates a:

- Multistage polytropic compressor
- Polytropic positive displacement compressor
- Isentropic compressor
- Isentropic turbine

MCompr has an intercooler between each compression stage. An aftercooler following the last compression stage is optional. The coolers can have liquid knockout outlet streams. You can introduce feed streams between stages. A variety of specification options are available for both the compression and cooling stages.

Pipeline

Pipeline calculates the pressure drop and heat transfer in a pipe segment or a pipeline. Pipeline can model any number of segments to describe the pipe geometry.

Pipeline handles a single inlet and outlet material stream. Pipeline assumes the flow is one-dimensional, steady-state, and fully developed (no entrance effects are modeled).

Pipeline can perform one- or two-phase calculations.

If the inlet pressure is known, Pipeline calculates the outlet pressure. If the outlet pressure is known, Pipeline calculates the inlet pressure and updates the inlet stream.

Pipe

Pipe calculates the pressure drop and heat transfer in a single pipe segment or annular space. Multi-phase, one-dimensional, steady-state and fully developed pipeline flow with fittings can be modeled.

Valve

Valve calculates the pressure drop or valve coefficient (C_V) for a control valve. Multi-phase, adiabatic flow in ball, globe and butterfly valves can be modeled.

Manipulators

Stream manipulators modify or change stream variables for convenience. They do not represent real unit operations.

Mult

Mult multiplies streams by a factor you specify. The heat and material balances are not maintained. The outlet stream has the same composition and properties as the inlet.

Dupl

Dupl copies the inlet stream to any number of outlet streams. This model does not satisfy material and energy balances. Dupl is useful for simultaneously processing a given stream in different types of units.

ClChng

ClChng changes the class of streams between blocks and flowsheet sections. It copies substreams from the inlet stream to the corresponding substreams of the outlet stream.

Solids

This table shows the solids models are what they do:

This model	Models
CCD	Multistage solids washers that recover dissolved components from an entrained liquid of a solids stream
CFuge	The separation of liquids from solids
Crystallizer	A mixed suspension, mixed product removal (MSMPR) crystallizer.
Crusher	Breaking solid particles in a crusher
Cyclone	Solids separation from a gas stream
ESP	Solids separation from a gas stream
FabFl	Solids separation from a gas stream
Filter	The separation of liquids from solids

Continued

This Model	Models
HyCyc	The separation of liquids from solids
Screen	Separating solid particles in a screen
SWash	Solids washers that recover dissolved components from an entrained liquid of a solids stream
Vscrub	Solids separation from a gas stream

Crystallizer

Crystallizer models a mixed suspension, mixed product removal (MSMPR) crystallizer. It performs mass and energy balance calculations. You have the option of determining the crystal size distribution.

Crystallizer assumes that the product magma leaves the crystallizer in equilibrium. The mother liquor in the product magma is saturated.

The feed to Crystallizer mixes with recirculated magma and passes through a heat exchanger before it enters the crystallizer. The product stream from Crystallizer contains liquids and solids. You can pass this stream through a hydrocyclone, filter, or other fluid-solid separator to separate the phases. Crystallizer can have an outlet vapor stream.

Crusher

Crusher simulates the breaking of solid particles.

Crusher models the wet or dry continuous operation of:

- Gyratory jaw crushers
- Single-roll crushers
- Multiple-roll crushers
- Cage mill impact breakers

Crusher assumes the feed is homogeneous. The breaking process creates fragments in the outlet solids stream with the same composition as in the feed stream.

Crusher does not account for heat produced by the breaking process.

Screen

Screen simulates the separation of various sizes of solid particles in a mixture. Each of the two outlet streams contain particles of a more uniform size.

Screen calculates the separation efficiency of the screen from the sizes of screen openings you specify.

FabFl

FabFl simulates baghouse fabric filter units.

A baghouse has a number of cells. Each cell contains a vertically-mounted, cylindrical fabric filter bag. The filter bags work in parallel to separate solid particles from a gas stream. Use FabFl to rate or size baghouses.

Cyclone

Cyclone simulates cyclone separators. Cyclone separators remove solid particles from a gas stream using the centrifugal force of a gas vortex.

Use Cyclone to size or rate cyclone separators.

VScrub

VScrub simulates venturi scrubbers.

Venturi scrubbers remove solid particles from a gas stream by direct contact with an atomized liquid stream.

Use VScrub to rate or size venturi scrubbers.

ESP

ESP simulates dry electrostatic precipitators.

Dry electrostatic precipitators separate solids from a gaseous stream. Electrostatic precipitators have vertically mounted collecting plates with discharge wires. The wires are parallel and positioned midway between the plates. The corona discharge of the high-voltage wire electrodes first charges the solid particles in the inlet gas stream. Then the electrostatic field of the collecting plate electrodes removes the solids from the gas stream.

Use ESP to size or rate electrostatic precipitators.

HyCyc

HyCyc simulates hydrocyclones. Hydrocyclones separate solids from the inlet liquid stream by the centrifugal force of a liquid vortex. Use HyCyc to rate or size hydrocyclones.

CFuge

CFuge simulates centrifuge filters. Centrifuge filters separate liquids and solids by the centrifugal force of a rotating basket. CFuge assumes the separation efficiency of the solids equals 1, so the outlet filtrate stream contains no residual solids. Use CFuge to rate or size centrifuge filters.

Filter

Filter simulates continuous rotary vacuum filters. Filter assumes the separation efficiency of the solids equals 1, so the outlet filtrate stream contains no residual solids. Use Filter to rate or size rotary vacuum filters.

SWash

SWash models the separation of solid particles from an entrained liquid of a solids stream.

SWash does not consider a vapor phase.

CCD

CCD simulates a counter-current decanter or a multistage washer. CCD calculates the outlet flow rates and compositions from:

- Pressure
- Mixing efficiency
- Number of stages
- The liquid-to-solid mass ratio of each stage

CCD can calculate the heat duty from a temperature profile. CCD does not consider a vapor phase.

User Models

User and User2 allow you to write your own unit operation models.

These models can simulate any unit operation model. You must write a Fortran subroutine to calculate the values of outlet streams, based on the inlet streams and parameters you specify.

See *Aspen Plus User Models* for detailed information about writing your own unit operation models.

Specifying Unit Operation Models

For each unit operation block, you must enter specifications on Block forms. To access these forms:

1. Select the block on the graphical flowsheet.
2. Click the right mouse button on the block.
3. From the popup menu that appears, click Input.
4. Select the appropriate form and sheet.

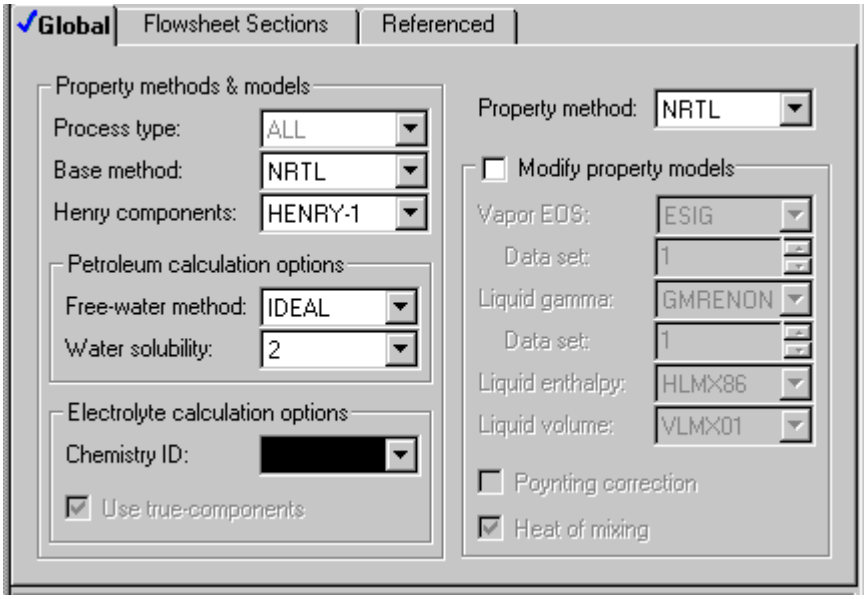
Overriding Global Specifications for a Block

You can use the BlockOptions form for a block to override global values for the following parameters:

Option	Specify globally on sheet	Specify locally on Block sheet
Physical Property Method, Henry's Components	Properties Specifications Global	BlockOptions Properties
Simulation Diagnostic Message Level	Setup Specifications Diagnostics	BlockOptions Diagnostics
Physical Property Diagnostic Message Level	Setup Specifications Diagnostics	BlockOptions Diagnostics
Stream Diagnostic Message Level	Setup Specifications Diagnostics	BlockOptions Diagnostics
Heat Balance Calculations	Setup Simulation Options Calculations	BlockOptions Simulation Options
Use Results from Previous Convergence Pass	Setup Simulation Options Calculations	BlockOptions Simulation Options
Valid Phases	Setup Specifications Global	Input Specifications

Example of Replacing a Global Properties Specification

Use the NRTL Method with Henry1 (Henry's Components) instead of the global values in Base Method and Henry's Components specified on the Properties Specifications Global sheet.



Requesting Heating/Cooling Curve Calculations

Many unit operation models can generate heating/cooling curves.

These curves calculate the following at intermediate points between the inlet and outlet conditions of a block, including phase transition points (bubble and dew points):

- Temperature
- Pressure
- Vapor fraction
- Heat duty
- Optional additional properties

To request heating/cooling curves for a block:

1. From the Data Browser tree for the block, select the Hcurves folder.
2. In the Hcurves Object Manager, click New.
3. In the Create New ID dialog box, enter an ID or accept the default ID. The ID must be an integer.

4. Select an independent variable:

- Heat Duty
  - Temperature
  - Vapor Fraction

  The selected variable is varied to generate the intermediate points.

5. To define the intermediate points, specify one of the following:

What to specify	Where
Number of points	Number of Data Points
Size of the increment between points	Increment Size
List of values for the independent variable	List of Values

If you specify Number of Data Points, the intermediate points will be equally spaced between the inlet and outlet.

6. Select the pressure profile option in the Pressure Profile frame. Specify Pressure Drop, if needed for the selected Pressure Profile option.

All of the pressure profiles are either constant or linear from the first pressure point to the last pressure point. This table shows the points used for each option:

Pressure Profile Option	First Point	Last Point
Constant	Outlet pressure	Outlet pressure
Linear	Inlet pressure - Pressure drop	Outlet pressure
Linear2	Inlet pressure	Inlet pressure - Pressure drop
Linear3	Outlet pressure + Pressure drop	Outlet pressure
Outlet	Outlet pressure	Outlet pressure
Inlet	Inlet pressure	Inlet pressure
Mid-point	(Outlet pressure + Inlet pressure)/2	(Outlet pressure + Inlet pressure)/2

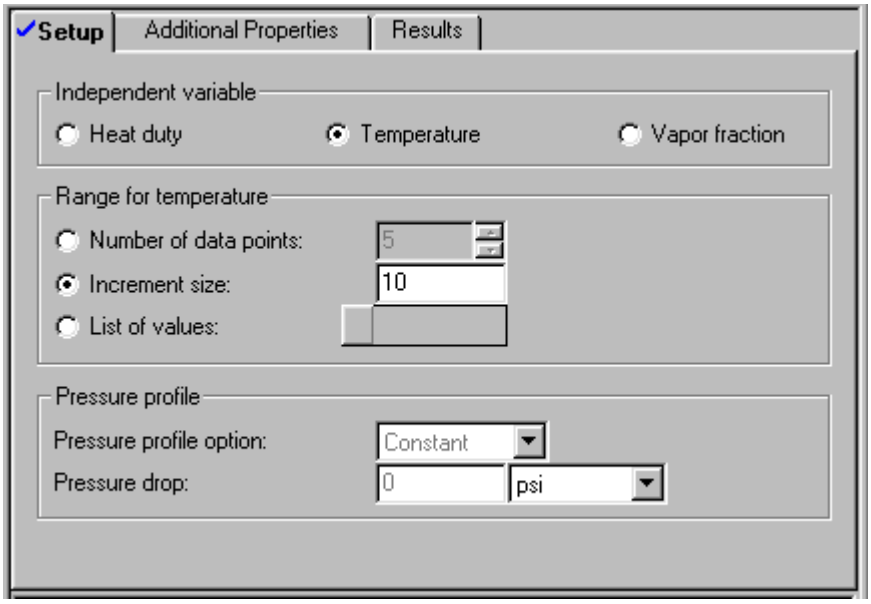
You can request additional properties to be calculated on the Additional Properties sheet. Any number of the Property Sets in the Properties Prop-Sets folder are available.

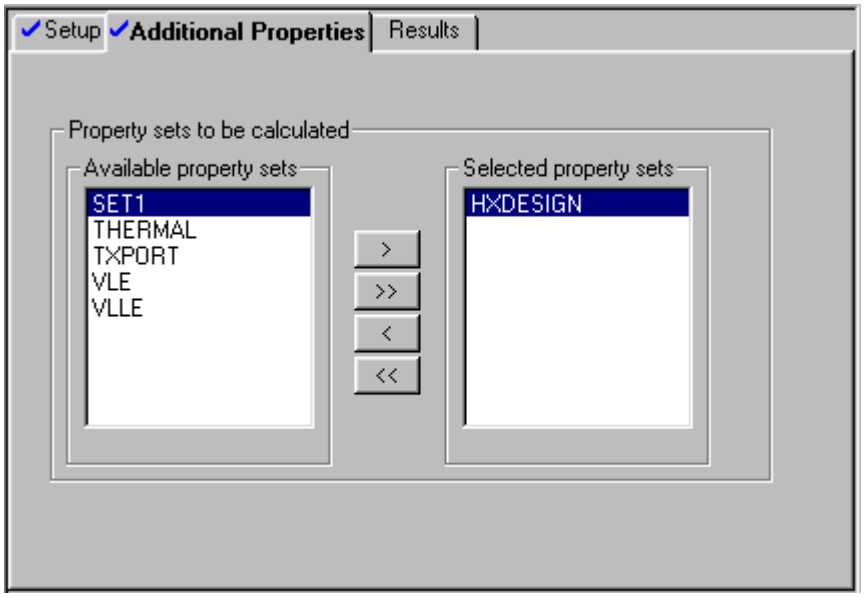
7. Select a Property set and click the left arrow to move the Property Set between the Available Property Sets list and the Selected Property Sets list. To move all of the property sets at once from one list to the other, click the appropriate double arrow.

If you will be using this heating/cooling curve for heat exchanger design, select the built-in property set HXDESIGN. HXDESIGN calculates all of the properties needed by design programs from HTRI, HTFS, and B-JAC. Aspen Plus includes an interface program, HTXINT, for transferring heating/cooling curve results to these programs. For information on how to use HTXINT, see Chapter 39.

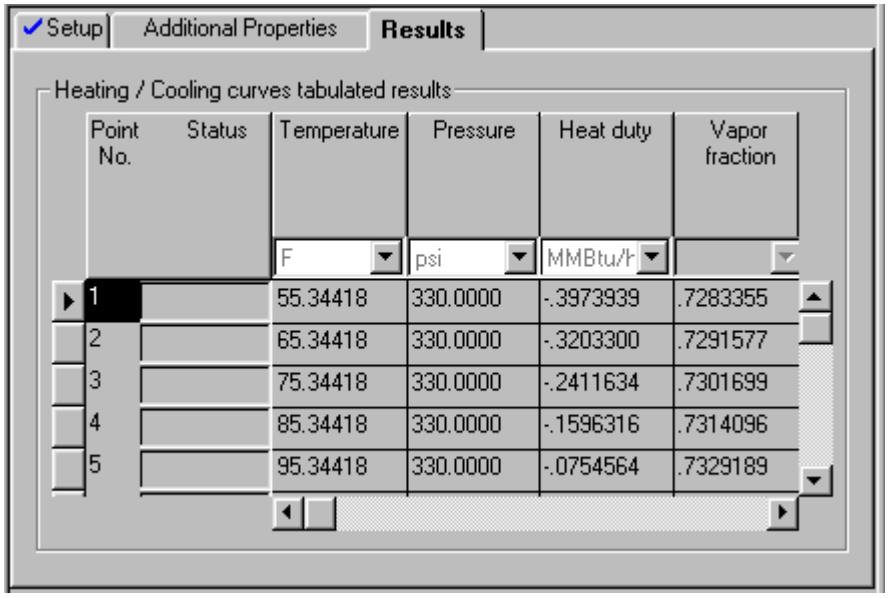
Example of Requesting a Heating Curve

Generate a heating curve that includes heat exchanger design properties. Points are generated every ten degrees.

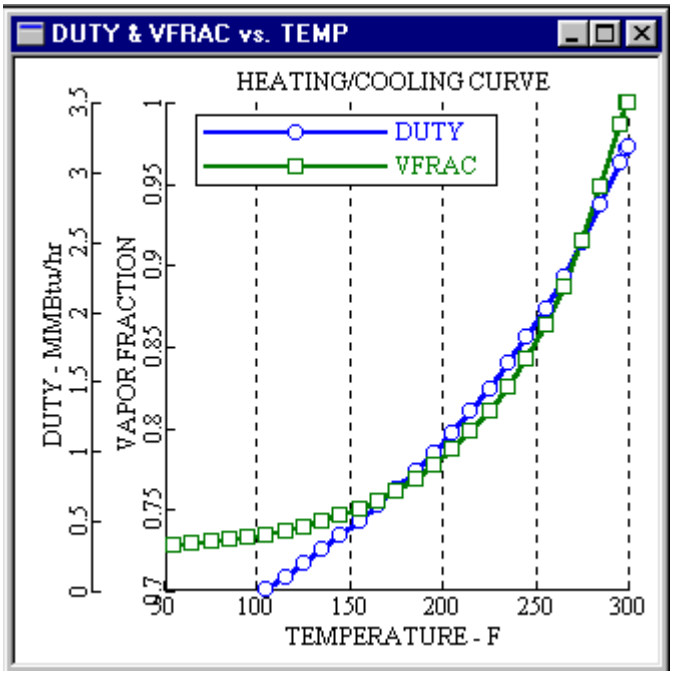




A table of data is generated after the simulation has been run.



A plot can be generated from the results.



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11 Running Your Simulation

This chapter describes how to run your simulation including:

- Running the simulation interactively
- Reinitializing simulation calculations
- Viewing the run status of the simulation
- Checking simulation history
- Running the simulation on the Aspen Plus host computer
- Running a simulation in batch (background) mode
- Running Aspen Plus in standalone (text only) mode
- Specifying run settings and user databanks

When your problem specifications are complete, you are ready to run the simulation. The status of your specifications is shown at all times in the status bar of the main window and the Data Browser. You can run your simulation if the status is any of these:

- Input Complete
- Input Changed
- Ready to Execute Block

You can run your simulation in these ways:

Type of Run	Information
Interactive	When you run interactively you control the simulation completely. You can step through the simulation, stop at any point, view any intermediate results, and make changes.
Batch (background) mode	When you run batch you cannot control the simulation. Batch simulations are useful for long simulations or when you want to run several simulations (case studies) simultaneously.
Standalone Aspen Plus (text only) mode	Standalone runs are similar to batch runs, but are made outside of the user interface.

Running the Simulation Interactively

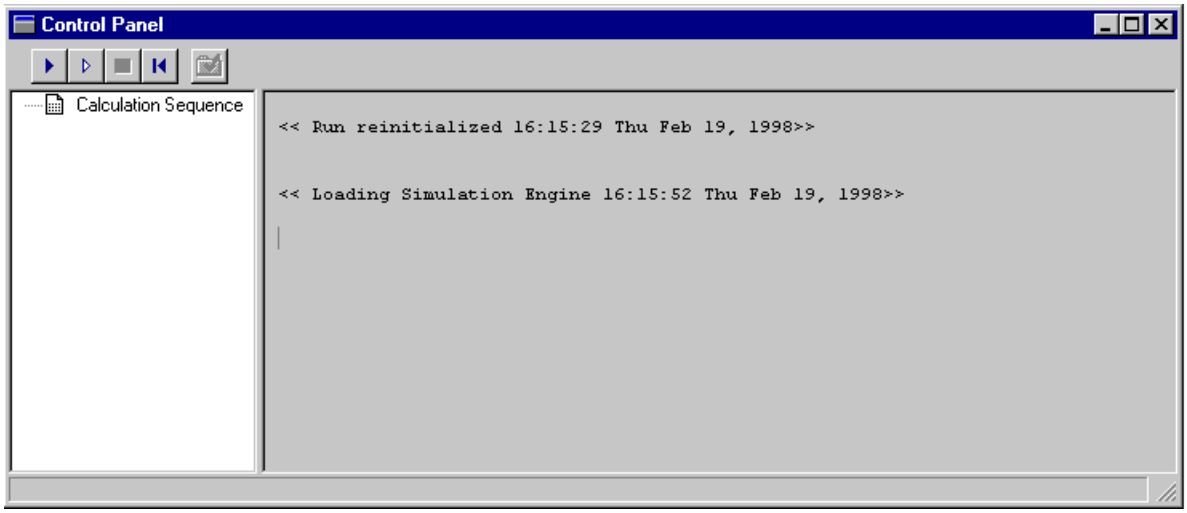
You can interactively control the simulation execution by using:

- The Run buttons on the Simulation Run toolbar
- The Run menu

You have the same flexibility in controlling the simulation whether the simulation engine is on your local computer or on a remote computer.

You can modify any input specifications at any time before or after a simulation, or when a simulation is paused.

You can view the progress of the simulation and control using the Control Panel.



The Control Panel consists of:

- A message window showing the progress of the simulation by displaying the most recent messages from the calculations
- A status area showing the hierarchy and order of simulation blocks and convergence loops executed
- A toolbar which you can use to control the simulation

Commands for Controlling Simulations

You can control the simulation by using the commands on the Run menu, the Simulation Run toolbar, or the Control Panel:

To	Do this
Start or continue calculations	Click the Start button  on the toolbar. – or – From the Run menu, click Run.
Pause simulation calculations	Click the Stop button  on the toolbar. – or – Click anywhere while the cursor is a stop sign.
Step through the flowsheet one block at a time	Click the Step button  on the toolbar. – or – From the Run menu, click Step.
Set stop points in the simulation	From the Run menu, click Stop Points. – or – On the Control Panel, select the block, click with the right mouse button, and select Stop Point Before or Stop Point After.
Change the next block to be executed	From the Run menu, click Move To. – or – On the Control Panel, select the block, click with the right mouse button, and select Move To.
Update results	From the Run menu, click Load Results to load all results from the simulation engine if Interactive Load Results is: Off and you stopped the simulation On and you want to load all results at one time For more information, see Changing Run Settings and User Databanks on page 11-11.
Check simulation results	Click the Check Results button  on the toolbar. – or – From the Run menu, click Check Results – or – In the left pane of the Data Browser, click the Results Summary form.
Display block or stream results	1. On the flowsheet, click the block or stream. 2. Then click with the right mouse button on the block or stream. 3. From the popup menu that appears, click Results.
Purge simulation results	Click the Reinitialize button  on the toolbar. – or – From the Run menu, click Reinitialize.

Changing Interactive Simulation Speed

When running interactively you can usually increase the speed of the calculations by selecting the Express Run option. For more information, see Changing Run Settings and User Databanks on page 11-11.

When the Express Run option is on, you cannot monitor the progress of the simulation while it is running. However, once the simulation is complete or stopped, you can check the Simulation History to see the progress and diagnostic messages.

Reinitializing Simulation Calculations

When you change your simulation specifications, by default, Aspen Plus uses any previously generated results as a starting point the next time you run the simulation. You can override this default by reinitializing the entire simulation, or specific blocks in the flowsheet, before rerunning the simulation.

To reinitialize before rerunning a simulation:

1. From the Run menu, click Reinitialize.
2. Choose the items you want to reinitialize in the Reinitialize dialog box.

Tip You can also do this from the Control Panel. Select the block or item, click with the right mouse button and click Reinitialize.

You may need to reinitialize if a block or the flowsheet:

- Fails to converge for no apparent reason, after you changed the block or specifications that affect its inlet streams
- Has multiple solutions and you can obtain the one you want only by starting from your specified initial block or stream estimates

Viewing the Status of the Simulation

You can view the progress of a simulation in:

- The Status Bar
- Control Panel Status Messages

Viewing Simulation Status Using the Status Bar

The main window status bar shows the progress of a running simulation and the current status of the simulation when it is not running. Status messages appear on the right side of the status bar.

This table shows the meaning of the status messages:

Status message	Meaning
Flowsheet Not Complete	Flowsheet connectivity is incomplete. To find out why, click the Next button in the toolbar.
Required Input Not Complete	Input specifications for the run are incomplete. Click Next on the toolbar to find out how to complete the input specifications, and to go to sheets that are incomplete.
Required Input Complete	The required input specifications for the run are complete. You can run the simulation or enter optional specifications.
Ready to Execute Block	The simulation is paused because you clicked the Stop or Step buttons, or a stop point you set was encountered. Click the Step or Run buttons to continue calculations.
Results Present	The run has completed normally, and results are present.
Results With Warnings	Results for the run are present. Warning messages were generated during the calculations. See the Control Panel for messages.
Results With Errors	Results for the run are present. Error messages were generated during the calculations. See the Control Panel for messages.
Input Changed	Results for the run are present, but you have changed the input since the results were generated. The results may be inconsistent with the current input.

Viewing Simulation Status Using the Control Panel Status Messages

The Control Panel message area contains progress, diagnostic, warning, and error messages generated during calculations.

This table shows the message and the information that follows it:

Control Panel Message	Information Displayed Following the Message
Processing input specifications	Flowsheet analysis for tear streams and calculation sequence. Errors associated with input specifications.
Calculations begin	Identification of each block as it is calculated. Iteration-by-iteration status of convergence blocks, and of column convergence. Errors during simulation calculations.

Continued

Control Panel Message	Information Displayed Following the Message
Generating results	Errors during the generation of results (heating and cooling curves, stream properties, property tables and any block calculations that were not needed during the simulation calculations).
Problem specifications modified	New flowsheet analysis for tear streams and calculation sequence, caused by flowsheet modifications. Errors associated with modified input specifications.

Checking the Status of Calculations

Use the Results Summary sheet to check the status of calculations. To do this:

1. On the Simulation Run toolbar, click the Check Results button  .

   – or –

   From the Run menu, click Check Results.

2. Click the Results Summary sheet.

   The Results Summary sheet appears. This sheet indicates whether the calculations were completed normally and shows error or warning messages resulting from the calculations.

   To see error and warning messages for a specific object, click the Status button  on the Data Browser toolbar when the forms for that object are displayed.

   For more information on checking the completion status of a run, click here. see Chapter 12.

Checking the Simulation History

Aspen Plus keeps a detailed history of your simulation run in a file that you can view with your text editor. Input specifications, warning messages, error messages, and block-by-block convergence information are available.

This table shows your options:

To	Do this
View the history of the current run	From the View menu, click History.
Save history to a file	Use the save command for your text editor.
Return to Aspen Plus	Use the exit command for your text editor.

Aspen Plus displays all results in the simulation history in SI units.

Running the Simulation on the Aspen Plus Host Computer

If your network configuration and your Aspen Plus license permits, you can run the Aspen Plus user interface on one computer and run the simulation engine on a different computer (the remote Aspen Plus host).

You may be required to connect to a remote Aspen Plus host when you start Aspen Plus. For more information on connecting to a host computer, see Chapter 1.

To change the Aspen Plus host computer after you have started Aspen Plus:

1. From the Run menu, click Connect to Engine.
2. In the Connect to Engine dialog box, enter the Server Type.

   If you choose your Local PC Host as the Aspen Plus host computer, you do not need to enter any more information into the dialog box.
3. For all Aspen Plus host computers except the PC, enter the following information in the dialog box:

In this field	Enter this information
Node Name	Node name of the computer the Aspen Plus simulation will run on
User Name	Your Logon name on the host computer
Password	Password for your account on the host computer
Working Directory	Working directory on the host computer for Aspen Plus runs

   Aspen Plus creates files for the run in the Working Directory. Specify the directory as you would in an operating system command. For example:

   To specify an OpenVMS subdirectory named SIMULATION, enter [.SIMULATION]. The default Working Directory is your home directory for that particular operating system.
4. Click OK.
5. When the network connection is established, a message box appears saying Connection Established.

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

Communicating with a Remote Aspen Plus Host Computer

You can use several commands to communicate with a remote Aspen Plus host computer simulation engine:

To	Do This
Check the status of a batch run	From the Run menu, select Batch, then Jobstat, and select the ID of the run you want information on.
Retrieve results from a batch run	From the Run menu, point to Batch, then Load Results, and select the ID of the run for which you want to retrieve results.

Running a Simulation Batch (Background)

There are times when you may not want to run the simulation interactively. For example, when you use a Sensitivity block or an Optimization block, or if the simulation is lengthy. In these cases you can submit a batch run.

Tip To avoid inconsistent input and results, do not change the input specifications for a run after you have submitted a batch run, until you have read back the results.

To start a batch run:

1. On the Run menu, select Batch, then Submit.
2. Use the check box to specify whether or not you want to delete the temporary files Aspen Plus generates after the run finishes.
3. You can specify Command Line Qualifiers, for the operating system (such as batch queue name), and for Aspen Plus (such as user databank filenames). You also can specify a working directory on the remote host in the Batch Submit dialog box. The default directory is your home directory on the remote host computer.
4. Click the Settings button if you want to change any run settings.
5. Click OK.

   Aspen Plus submits the batch run.

To check the status of the batch run:

↘ From the Run menu, point to Batch, then Jobstat.

After the batch run is finished, you can load the results into the user interface. To load the results into the interface:

1. From the Run menu, point to Batch, then Load Results.
2. Select the ID of the run for which you want to retrieve results.

Running Aspen Plus Standalone

You can use the Aspen Plus user interface to develop the simulation model for a run and view the results, but run the Aspen Plus simulation engine separately from the user interface. You might want to do this to achieve maximum performance for large flowsheets.

To run the Aspen Plus simulation engine standalone:

1. Complete the input specifications for the run in the user interface. When the status indicator in the main window toolbar says *Required Input Complete* or *Input Changed*, you can run the simulation.
2. From the File menu, click Export.
3. In the Save As Type field, select Input File (.inp). Enter the Run ID for the filename.
4. If you are running the simulation engine on a remote computer, transfer the file **`runid.inp`** to the remote computer.
5. From the operating system prompt, enter the command:

   `aspen runid`

6. If you are running the simulation engine on a remote computer, transfer the file **`runid.sum`** from the remote computer to the local computer when the run is complete.
7. When the run is complete, from the File menu, click Import and in the Files Of Type box, select Summary file (.sum).
8. From the file list, select the Run ID and click OK.
9. You can now review the results and modify the input in the user interface, as if you had made the run from within the user interface.

Editing the Input File for Standalone Runs

You can edit the input file outside the interface. The following instructions ensure that:

- Any changes you make in the input file are reflected in the user interface.
- Your graphical flowsheet will be restored when you return to the user interface.

To edit the Aspen Plus input file outside of the interface:

1. Complete the input specifications for the run in the user interface. When the status indicator in the main window toolbar says *Required Input Complete* or *Input Changed*, you can run the simulation.
2. From the File menu, click Export.
3. In the Save As Type field, select Input Files with Graphics (.inp). Enter the Run ID for the filename.
4. If you are running the simulation engine on a remote computer, transfer the file **`runid.inp`** to the remote computer.
5. Edit your input file to make the changes.
6. Use the aspen command option to create a backup file:

   aspen runid /mmbackup
7. If you are running the simulation engine on a remote computer, transfer the files **`runid.sum`** and **`runid.bkp`** to the local computer.
8. When the run is complete, start the Aspen Plus user interface.
9. From the File menu, click Open, and select Backup files (.bkp). Then select the Run ID from the file list.
10. Click OK.
11. From the File menu, click Import, and in the Files Of Type field, select Summary file (.sum).
12. Select the Run ID from the file list, and click OK.

Changing Run Settings and User Databanks

To display the Run Settings dialog box:

1. From the Run menu, click Settings.
2. On the Engine Files Tab, you can specify filenames for:

Item	Information
User physical property databanks	The property databanks are called USRPP1A, USRPP1B USRPP2A, USRPP2B and USRPP2C. For more information, see *Aspen Plus Physical Properties Data*.
User insert libraries and stream libraries	In Aspen Plus, when referring to insert libraries or stream libraries, you must use the file extension .ILB for insert libraries, and .SLB for stream libraries.
Link Options	The Dynamic Linking Options File (DLOPT) contains directives for dynamic linking. For more information, see *Aspen Plus User Models*.
Run Definition	The User defaults file is used to override system defaults files and specify default command options.
A user cost databank	The user cost databank is used to update the cost indices.

   These filenames apply when you run the simulation interactively or in batch.
3. On the Options tab, use the Express Run option to achieve maximum simulation speed when running the Aspen Plus simulation engine on a PC, or when running interactively on other platforms. The Express Run option:
   - Turns off the Animation option
   - Sets the Control Panel message levels to 0
   - Turns off interactively loading results
   - Enables you to use History from the View menu to examine the progress of a simulation

Interactively Load Results

By default, Aspen Plus results are loaded into the user interface only when you want to examine them.

To change whether Interactively Load Results is on or off:

1. From the Tools menu, click Options.
2. On the Run tab, check or clear Interactively Load Results.

Have Interactively Load Results	If	Then
On	You want Aspen Plus to load only the results you are interested in. (You can still load all results by using Load Results from the Run menu.)	Aspen Plus speeds up the processing time by only loading particular results. This is useful if you run a simulation several times, but are only interested in the results on one particular form.
Off	You want all results to be loaded automatically at the end of a run	Aspen Plus loads all simulation results into the user interface. This increases the time required for a run to complete, but enables you to examine results more quickly.

Note Interactively Load Results only works with the Flowsheet Run Type.

12 Examining Results and Generating Reports

- View simulation results interactively
- Checking the completion status of a run
- Checking the convergence status of a run
- Displaying stream results
- Generate an Aspen Plus report file

Viewing Simulation Results Interactively

You can view results whenever the status message in the bottom window status bar is one of the following:

Message	Means
Results Available	The run has completed normally, and results are present.
Results Available with Warnings	Results for the run are present. Warning messages were generated during the calculations. View the Control Panel or History for messages.
Results Available with Errors	Results for the run are present. Error messages were generated during the calculations. View the Control Panel or History for messages.
Input Changed	Results for the run are present, but you have changed the input since the results were generated. The results may be inconsistent with the current input.

Use the results status indicators, which appear in the Data Browser to guide you to forms and objects. For a complete list of the status indicators, see Chapter 1.

Viewing Current Simulation Results

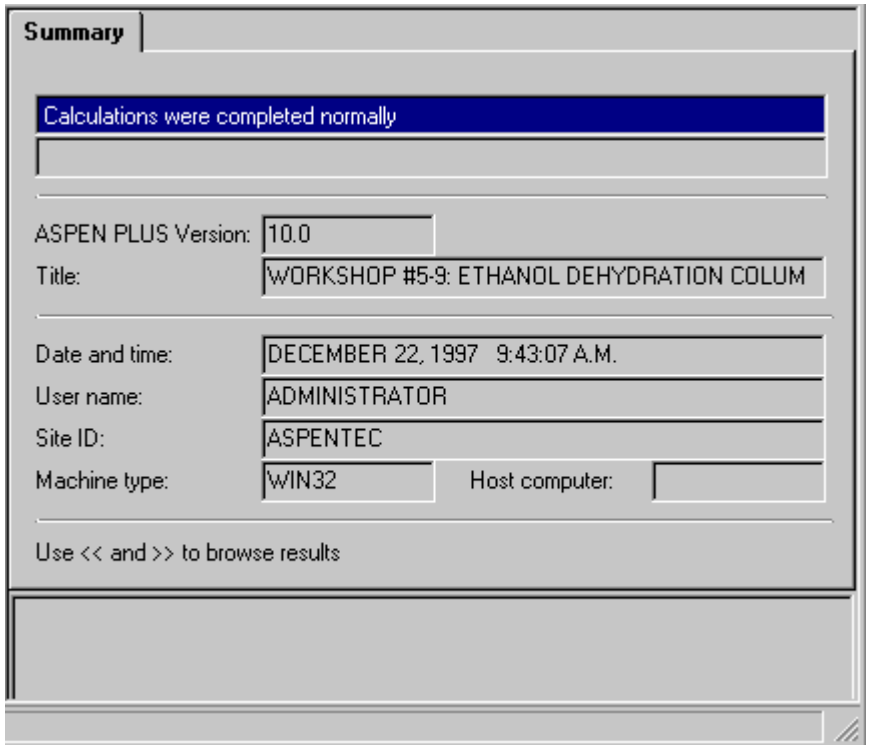
You can view the current simulation results after using the Stop or Step commands. To do this:

1. From the Run menu, click Settings.
2. In the Run Settings dialog box, ensure that the Interactively Load Results option is cleared.
3. From the Run menu, click Check Results.

Use the results status indicators, which appear in the Data Browser, to guide you to forms and objects with results.

Checking the Completion Status of a Run

Use the Results Summary sheet to examine summary information about the convergence and completion status of a run. This form indicates whether the calculations were completed normally.



To display the Results Summary sheet, do one of the following:

From the	Select
Simulation Run toolbar or the Control Panel	The Check Results button 
Data Browser	Results Summary in the left pane of the Data Browser
Run menu	Check Results

If errors or warnings exist:

1. When on a particular form, click the Status button  on the toolbar of the Data Browser window to see specific messages.
2. Check the Control Panel and History file for information, diagnostic, warning, and error messages generated during calculations.

Checking Completion Status in the Control Panel

The Control Panel displays error, warning and diagnostic messages from the run.

The number of messages can be controlled globally using the Setup Specifications Diagnostics sheet or locally using the block BlockOptions Diagnostics sheet.

The messages on the control panel are similar to those printed in the history file (*.his). The diagnostic level of the history file and the control panel can be adjusted independently.

If a high level of diagnostics is needed, the diagnostics should be printed to the history file and not to the control panel. This means you will not slow down performance by writing a lot of information to the screen.

To view the Control Panel, do one of the following:

From the	Select
View menu	Control Panel
Simulation Run toolbar	Show/hide control panel window button 

The Run Messages file (*.cpm) is a text file that includes all of the messages printed on the control panel. Run Messages files must be exported from the simulation to be saved. For more information, see Chapter 15.

Checking Completion Status in the History File

The History file displays error, warning and diagnostic messages from the run.

The number of messages can be controlled globally using the Setup Specifications Diagnostics sheet or locally using the block BlockOptions Diagnostics sheet.

To check the History file:

➤ From the View menu, click History.

A history file cannot be directly saved or exported from the Aspen Plus User Interface. However, the file is saved automatically when a run is saved as an Aspen Plus document (*.apw). You can also save the viewed history file using the text editor.

The history file is similar to the Run Messages file (*.cpm). The diagnostic level of the history file and the control panel can be adjusted independently. If a high level of diagnostics is needed, they should be printed to the history file and not to the control panel so as to not inhibit performance by writing so much information to the screen.

Checking the Convergence Status of a Run

Design specifications and tear streams both have associated convergence blocks. The Aspen Plus generated convergence block names begin with the character "$." User-defined convergence blocks must not begin with the character "$." For more information on Convergence, see Chapter 17.

Summary of Convergence Block Results

To see a summary of all of the convergence blocks for a run:

1. In the left pane of the Data Browser, click Results Summary, then select Convergence.
2. This table shows which sheets to use for summary information:

Select this sheet	For a summary of
DesignSpec Summary	The convergence status, final manipulated variable value, and final errors for all design specifications in the simulation
Tear Summary	The convergence status and final maximum errors for all tear streams in the simulation

Detailed Convergence Block Results

To see detailed results for a convergence block and its iteration history:

1. From the Data menu, point to Convergence, the click Convergence.
2. From the Convergence Object Manager, select a convergence block ID.
3. Click the Edit button.

   – or –

4. Double-click a convergence block ID.
5. From the Results form:

Select	To see
Summary	How tightly each tear variable or manipulated variable was converged
Spec History	The errors at each iteration. You can plot the iteration history.
Tear History	The maximum error at each iteration among all tear stream variables converged by this block. You can plot the iteration history.
Max Error/Tol	The maximum error divided by the tolerance at each iteration for all tear streams and design specifications.
Tear Variables	The value at each iteration of all tear stream variables converged by this block.

Displaying Stream Results

This table shows how to display stream results:

To display	Do this
A single stream	1. Click the stream. 2. Click with the right mouse button on the stream. 3. From the popup menu that appears, click Results.
The inlet and outlet streams of a block	1. Click the block. 2. Click with the right mouse button on the block. 3. From the popup menu that appears, click Stream Results.
All streams	From the Data Browser, point to Results Summary, then Streams.

On any Results Summary Streams sheet, click the down arrow in the Display box to select whether all stream or selected streams are displayed:

To add a stream to the display on any Results Summary Streams sheet:

1. Move to a field in the top row of a column.

2. Click the arrow to see a drop down list of streams.

To remove a stream from the display:

1. Click the stream ID.
2. Click the right mouse button.
3. From the popup menu that appears, click Clear.

This table shows which sheets display which results:

Select this Results Summary Stream sheet	To display
Material	Results for all or selected material streams in a spreadsheet format If you designate any batch streams, Aspen Plus displays the batch stream results (such as cycles/day, cycle time, down time). You can format the stream results, transfer the stream results to the Process Flowsheet as a table, or print the results. For more information, see Chapter 14 . For more information about stream summary formats, see Formatting Stream Results on page 12-7.
Heat	Heat flow results for all or selected heat streams in a spreadsheet format Aspen Plus uses heat streams to transfer duties to or from unit operation blocks.
Work	Power results for all or selected work streams in a spreadsheet format Aspen Plus uses work streams to transfer power to or from pumps or compressors.
Vol. % Curves	The Volume percent curves for all or selected streams. TBP curve, ASTM D86 curve, ASTM D1160 curve, Vacuum at 10 mmHg curve, API curve, and Specific gravity curve can be viewed. For more information, see Chapter 32.
Wt. % Curves	The Weight percent curves for all or selected streams. TBP curve, ASTM D86 curve, ASTM D1160 curve, Vacuum at 10 mmHg curve, API curve, Specific gravity curve, Molecular weight curve, and ASTM D86CRK curve can be viewed. For more information, see Chapter 32.
Petro. Curves	Petroleum property curves for all or selected streams. For more information, see Chapter 32.

Formatting Stream Results

The settings you specify on the Setup ReportOptions Stream sheet determine the contents of the Results Summary Streams Material sheet. For more information on specifying stream results, see Chapter 5.

The table format file (TFF) shown in the Format box of the Stream Summary sheet determines the format (order, labels, precision, and other options) of the stream results.

Aspen Plus provides built-in TFFs tailored to each Application Type. The default is an appropriate TFF for the Application Type you choose when you create a new run. You can also create your own TFFs. For more information on creating your own TFFs, see Chapter 36.

Choosing a Table Format File

To choose a TFF:

1. From the Data menu, click Results Summary, then Streams.
2. Click the Material sheet.
3. In the Format box, click the drop down arrow and select a TFF from the List.

   If you are using built-in TFFs, it is recommended that you select a TFF for your Application Type. For example, if you are using a Petroleum Application Type, choose a TFF beginning with PET.

Tips

You can also specify the TFF on the Setup ReportOptions Streams sheet. Aspen Plus uses the TFF you select for all Stream Summary sheets you display, until you select another TFF.

Some TFFs filter the calculated stream results. If you want to make sure you see all calculated properties, select TFF FULL.

Displaying Heat and Work Stream Results

To display results for heat and work streams, follow one of these procedures:

To display results for	Do this
A single stream	1. Click the stream 2. Click the right mouse button and from the popup menu that appears, click Results.
All streams	1. From the Data Browser, click Results Summary, then Streams. 2. Click the Heat or Work tab.

Generating a Report

You can generate a report file documenting the complete input specifications and simulation results for your Aspen Plus run. Use the Report Options forms to control report contents. For more information about report options, see Chapter 5.

Before generating a report, the results of an interactive run must be available. You need to make an interactive run if:

- You have not yet run the simulation.
- You changed input specifications since running the simulation.
- You changed settings on the Report Options forms since running simulation.
- You opened a run saved in backup format, and have not run the simulation in the current session.

To make an interactive Run:

➤ On the Simulation Run toolbar, click the Run button  .

– or –

➤ From the Run menu, click Run.

To generate a report:

➤ From the View menu, click Report.

Export a Report File

To save the entire report file from an interactive run:

1. From the File menu, click Export.
2. In the Save As Type box, select Report files.
3. Enter a filename. The file can be in any directory on the local computer.
4. Select Save to create the report file.

Aspen Plus generates a report automatically during a batch run. The filename is the Run ID, with the .rep extension. The report file for a batch run is saved on the computer running the Aspen Plus simulation engine. If Aspen Plus is running on a remote computer, the report file is saved on that computer's file system.

For more information on managing files, see Chapter 15.

Viewing a Section of the Report

To view the entire report or a selected portion of a report in a text editor:

1. From the View menu, click Report.
2. Select the part of the report that you would like to view:

Select	To display
Block	The results of a specified unit operation block
Convergence	The results of a specified Convergence block
Sensitivity	The results of a specified Sensitivity block
Transfer	The results of a specified Transfer block
Fortran	The results of a specified Fortran block
Streams	The results of a specified stream or of all streams
Balance	The results of a specified Balance block
Pressure Relief	The results of a specified Pressure relief block
Regression	The results of a specified Regression block
Simulation	The entire Report file
Table Of Contents	Table of contents for the report
Flowsheet Balance	Material and energy balance for the flowsheet
Connecting Streams	The connecting streams (feeds and products) for a selected block

3. If necessary, select the ID for the block, stream, or other object.
4. Click Apply to display your selection in the text editor.
5. Repeat steps 2-4 to display any additional sections of the report.
6. Click OK.

Tips

Any of the sections of the report can be saved or printed using the text editor.

Use Copy and Paste to copy results from any sheet into another Windows program.

13 Working with Plots

This chapter describes how to generate, customize, and print plots from any input or results sheet that has tabular data, including:

- Generating plots
- Working with plots
- Printing plots

About Plots

Aspen Plus plots are a useful way of viewing the date from a run. You can use plots to display:

- Input and results profiles for unit operation blocks
- The results of flowsheeeting options and model analysis tools such as Sensitivity, Optimization, and Pres-Relief.

There are three steps involved in generating a plot:

1. Displaying the sheet containing the data you want to plot. The sheet may contain either input or results data.
2. Generating the plot either by:
   - Using the Plot Wizard

   –or–

   - Selecting the dependent, independent, and parametric variables
3. Customizing the plot appearance.

Step 1: Displaying the Data

To display data:

1. From the Data menu, click Data Browser.
2. In the left hand pane, click the form containing the data that you want to plot.
3. On the form, click the sheet to display the data.

   This sheet can be either an input or a results sheet though it is much more common to plot results.

3. To plot results, make sure that the simulation run has results available.

   If results are available, the status message in the main window will be Results Available, Results Available with Warnings, Results Available with Errors, or Input Changed. For more information on status messages when results are present, see Chapter 12.

   If results are not available, run the simulation.

Step 2: Generating a Plot

You can generate the plot in either of these ways:

- Using the Plot Wizard
- Selecting the dependent and independent variables

Using the Plot Wizard

Use the Plot Wizard to generate a plot quickly by selecting from a list of predefined plots. The Plot Wizard is available for most blocks and other objects which have tables of results.

After you have displayed the data:

1. From the Plot menu, click Plot Wizard.

   Note The Plot menu is only visible when you have the Data Browser in the current window.

   The Plot Wizard Step 1 appears.

2. Click Next.
3. Select the type of plot from the list of available plots, then click Next.
4. Select the options for the plot type you have selected.

   The options that are available depend on the plot type selected.
5. Click Next.
6. Select the general options for the plot type you have selected.

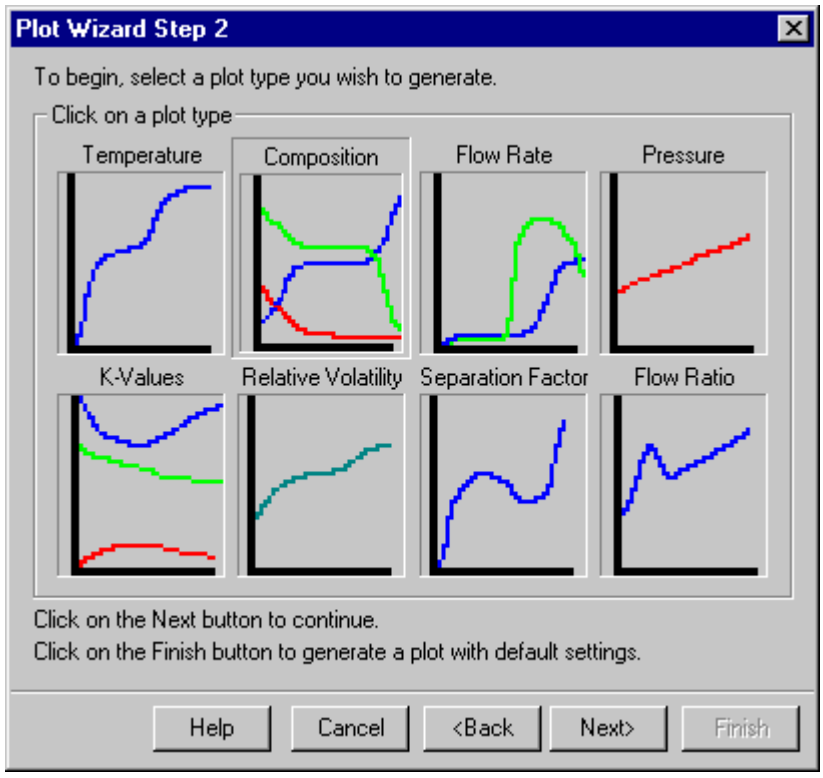
   The Plot Wizard guides you through the options. These include:

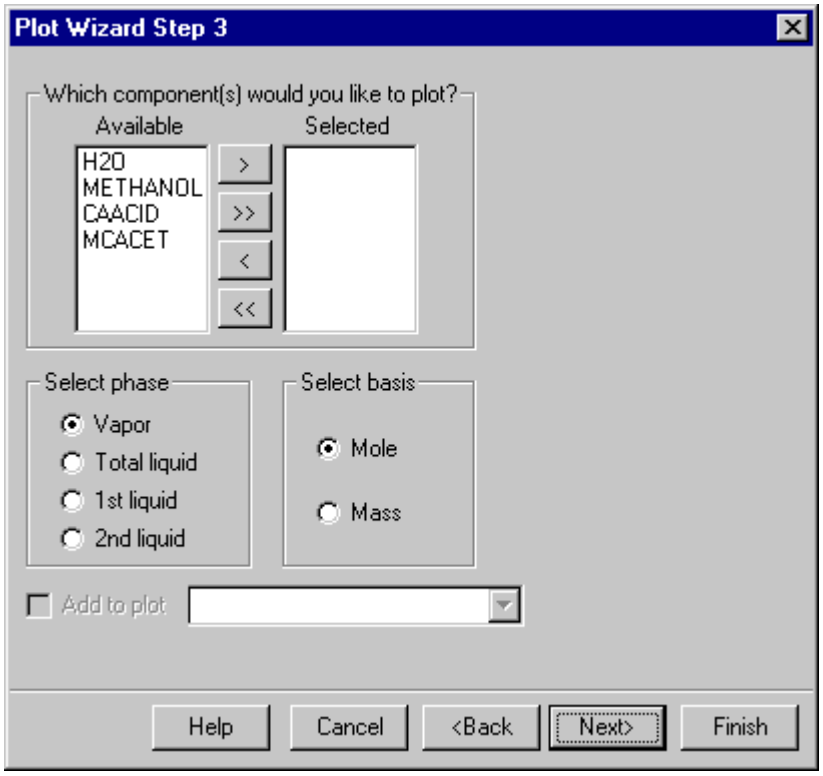
   - Changing the Plot type
   - Modifying the Plot and Axis titles
   - Choosing whether you want the plot updated when new results are available
   - Selecting if you want to display the plot legend
   - Adding a time stamp

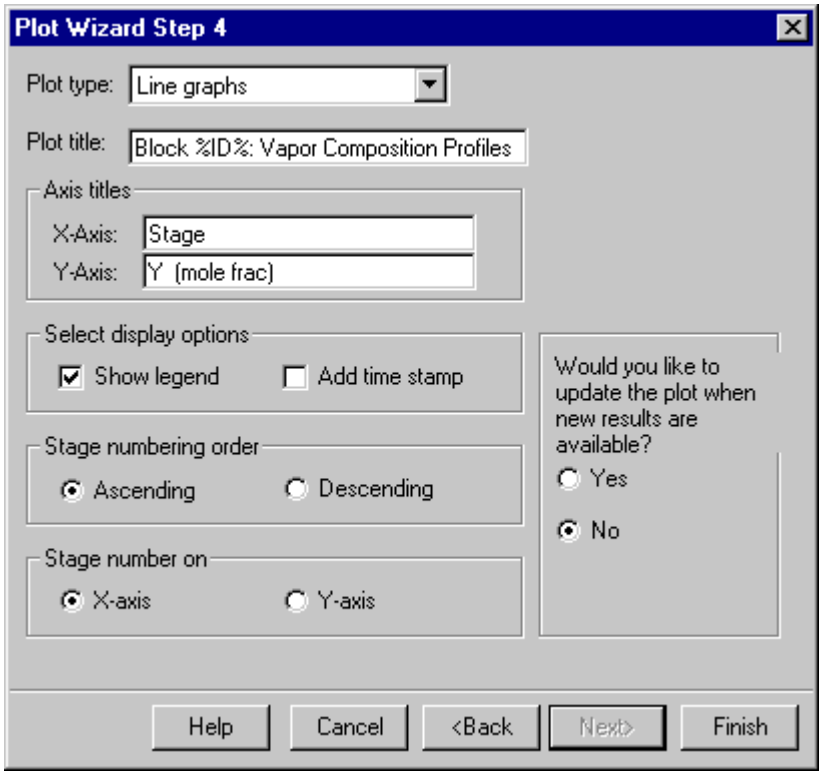
   For further details on these, see Step 3: Customizing the Appearance of a Plot on page 13-7.
7. To end the Plot Wizard and generate the plot, click Finish.

   For information on changing the plot attributes after exiting the wizard, see Step 3: Customizing the Appearance of a Plot on page 13-7.

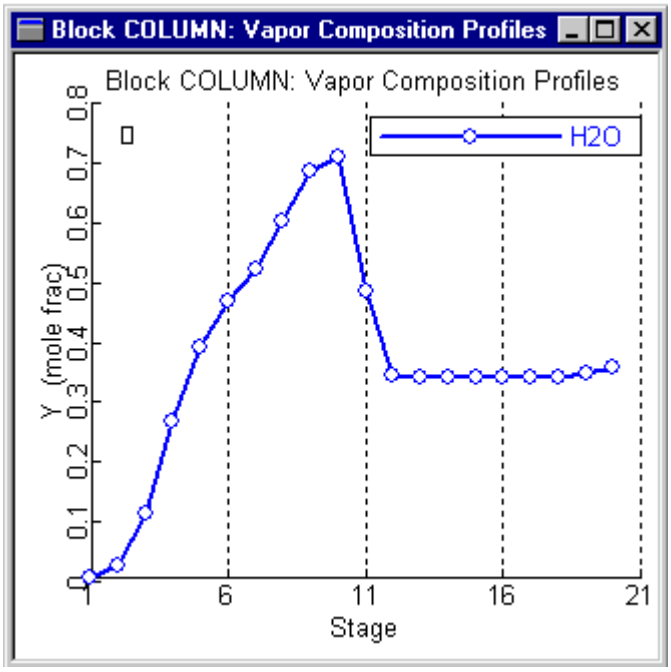
Example of Making a Plot of Flow Rate for a Radfrac Column




Plot Wizard Step 3
Which component(s) would you like to plot?
Available
Selected
H2O
METHANOL
CAACID
MCACET
>
>>
<
<<
Select phase
Vapor
Total liquid
1st liquid
2nd liquid
Select basis
Mole
Mass
Add to plot
Help
Cancel
<Back
Next>
Finish


Plot Wizard Step 4
Plot type:
Line graphs
Plot title:
Block %ID%: Vapor Composition Profiles
Axis titles
X-Axis:
Stage
Y-Axis:
Y (mole frac)
Select display options
Show legend
Add time stamp
Stage numbering order
Ascending
Descending
Stage number on
X-axis
Y-axis
Would you like to update the plot when new results are available?
Yes
No
Help
Cancel
<Back
Next>
Finish

The plot generated:



Generating a Plot by Selecting Variables

The Plot Wizard is usually the quickest way to generate a plot. However, if the plot you are interested in is not available in the Plot Wizard, you can generate the plot by selecting the independent, dependent, and parametric variables.

To select variables:

1. Click the title of the column of data you want to plot on the X-Axis.
2. From the Plot menu, click X-Axis Variable.
3. Select all the dependent variables:
   - Hold down Ctrl and click the title of each column of data you want to plot on the Y-Axis.
   - From the Plot menu, click Y-Axis Variable.
4. If you want to plot a parametric variable:

   Click the title of the column of data you want to plot as the parametric variable.
5. From the Plot menu, click Parametric Variable.

This table shows the types of variables available for a plot:

This variable	Is	You can
Y-Axis variable	The dependent variable	Select as many Y-Axis dependent variables as you like for a plot. You must select at least one Y-Axis dependent variable.
X-Axis variable	The independent variable	Select only one X-axis independent variable or accept the default independent variable (usually the first column of data)
Parametric variable	The third variable	Use this variable to plot a dependent variable against an independent variable for several values. For example, you might use a sensitivity block to generate a plot of reaction conversion (the dependent variable to be plotted on the Y-axis) versus residence time (the independent variable to be plotted on the X-axis) for three temperatures (the parametric variable).

Step 3: Customizing the Appearance of a Plot

You can customize the appearance of your plot by:

- Adding and modifying annotation text
- Changing the plot properties

Adding and Modifying Annotation Text

You can:

Do This	And
Add text to annotate a plot	The text can be attached or unattached.
Attach text to a point on a plot line	The text moves with the point as you zoom in and out and scroll through the plot workspace.
Place unattached text anywhere within the plot workspace	The text stays in the same place within the window as you zoom in and out and scroll through the workspace.

To add text to a plot:

1. Display the plot on which you want to add text.
2. Click the right mouse button on a plot and from the popup menu that appears, point to Modify, then click Add Text.

3. Use the Plot Text Setting dialog box to add or change the text.

Use this text sheet	To
Text	Enter the annotation text and specify color and orientation
Attribute	Attach the text to data point. You can connect it without an arrow or with a small, medium or large arrow. The default is to attach it with a medium arrow. Leave the text unattached. You can either left, center, or right justify it. The default is to left justify the text.
Font	Select the font, style and size for the text

4. Click OK.
5. Click the location on the plot where you would like to have the text placed.
6. If the text is attached to a data point, Aspen Plus automatically draws a line to the nearest curve. If this location is not desired, the point of attachment can be selected and dragged to any point on any curve in the plot.

To modify text on a plot:

1. Select the text that you want to modify. It will be highlighted once it is selected.
2. Click the right mouse button and click Edit.
3. Use the Plot Text Settings dialog box to change the text.
4. Click OK.

You can also change the default text font on a plot. For information on changing plot defaults, see Changing Plot Defaults on page 13-17.

Changing Plot Properties

Most of the elements of a plot can be modified using the Plot Control Properties dialog box. To access this dialog box:

➤ Double-click the plot.

– or –

Click the right mouse button over the plot and from the menu that appears, click Properties.

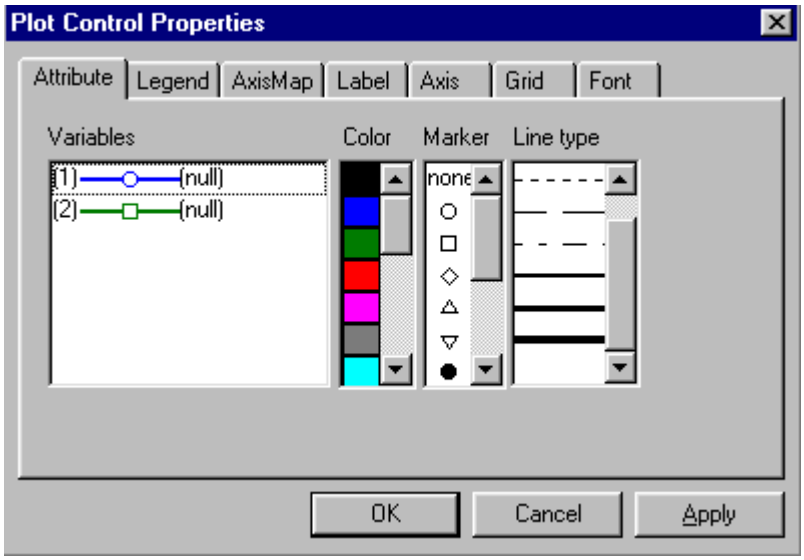
The following sections describes the changes you can make to a plot.

Changing Plot Attributes

You can change the appearance of data lines on a plot. The color, line, type and marker type can be modified for each variable.

To change the attributes of the data lines on the plot:

1. Display the plot.
2. Click the right mouse button on the plot and from the menu that appears, click Properties.
3. Click the Attribute tab.
4. Select the variable.
5. Select the Color, Marker, and Line type for that variable.



Displaying the Plot Legend

To show a legend on a plot:

1. Display the plot.
2. Click the right mouse button on the plot and from the popup menu, point to Modify, then click Show Legend.

Modifying the Plot Legend

You can modify the legend text and font:

1. Display the plot.
2. Double-click the legend.

   – or –

   When the cursor is positioned over the legend, click the right mouse button and then click Edit.
3. On the Plot Legend dialog box, click the line of the legend that you want to change and it appears in the Legend Text box.
4. In the Legend Text box, change the legend.
5. Click Replace.
6. Repeat steps 3–4 for every line of the legend that you want to change.
7. On the Font tab, you can modify the font for the entire legend.

   The legend can be hidden and then revealed, and all changes to the legend will be preserved.

   You can also change whether a legend appears by default on your plots. For information on changing plot defaults, see Changing Plot Defaults on page 13-17.

Changing the Axis Map

If a plot has more than one dependent variable, by default Aspen Plus displays the plot with a separate Y axis scale for each dependent variable. You can map all variables to a single axis, or you can map groups of variables to designated axes.

For example, if you plot column mole fraction profiles for five components, you can plot all components against a single Y axis scale. If you plot temperature, liquid rate and vapor rate on the same plot, you can plot temperature on one axis and both flow rates on another.

To specify axis mapping:

1. Display the plot.
2. Click the right mouse button on the plot and from the popup menu, click Properties.
3. Click the AxisMap tab.
4. Select a dependent variable.
5. This table shows what you can do:

Use	To
The Up and Down arrows	Change the axis number the variable is mapped to. If you reduce an axis number to zero, the plot of the dependent variable is not displayed.
The All in One button	Map all dependent variable to a single axis.
The One for Each button	Map each dependent variable to a separate axis.

6. Click OK.

Changing Plot Titles

You can change the text on the plot titles at any time by customizing the font, style, and size for the text.

To change the plot title for a specific plot:

1. Display the plot that you want to change.
2. Double-click the title that you want to change.
3. On the Text tab, enter the text for the title.
4. On the Font tab, select the font, style, and size for the text.

   You can also change the default text font for plot titles. For information on changing plot defaults, see Changing Plot Defaults on page 13-17.

Changing Plot Axis Labels

The text on the plot axis labels can be modified at any time. The font, style, and size for the text can also be customized for each label.

To change the plot axis labels for a specific plot:

1. Display the plot.
2. Double-click the axis label that you want to change.
3. On the Text tab, enter the text for the axis label.
4. On the Font tab, select the font, style, and size for the text.
5. Repeat steps 2–4 for any other axes that you wish to modify.

   You can also change the default font for all plot axis labels. For information on changing plot defaults, see Changing Plot Defaults on page 13-17.

Changing Plot Axes

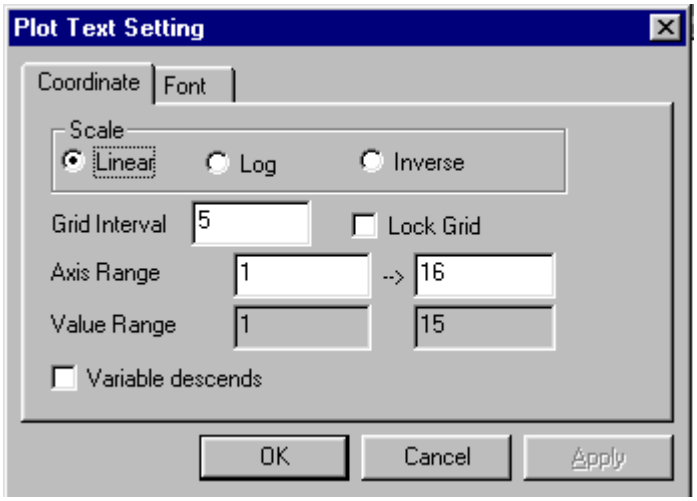
The scale options for the X and Y axes can be changed in order that a specific area of the plot can be viewed. If a plot has more than one Y axis scale, the scale for each one can be changed separately.

To change scale options for the X or Y axis:

1. Display the plot.
2. Double-click the Axis values that you want to change.
3. Select whether you want a linear, log or inverse scale.
4. Change the Grid interval.

   – or –

   To return to the automatic grid interval determined by Aspen Plus, turn off the Lock grid option.
5. Use the Axis Range settings to plot only a subset of the data, or to specify endpoints for the axis scale. To return to the automatic range determined by Aspen Plus, delete the entries from the Range text boxes.
6. The Value Range boxes (displayed below the Axis Range boxes) show the range of data.
7. If you want to invert the axis to display the variable values decreasing from the origin, check the Variable Descends box.
8. On the Font tab, select the font, style and size for the text.



Changing the Grid Display for a Plot

To change the grid and line display options for a specific plot:

1. Display the plot.
2. Double-click the plot background.
3. Click the Grid tab.
4. Change the options desired.

   This table shows the display settings that you can change:

Choose this Plot Option	To
Grid	Define the type of grid for the plot. Choose from: Mesh (Horizontal and vertical grid) Horizontal Vertical No grid
Line	Select the line style for the data curves. Choose from: Lines & markers Lines Markers
Flip coordinate	Flip the x and y axes
Square plot	Set the range of the x and y axes to be the same
Diagonal line	Draw a diagonal line where x=y on the plot
Zero line	Draw a horizontal line at the zero point of the x axis
Marker size	Modify the size of the markers displayed in the plot

You can also change the default display options for plots. For information on changing plot defaults, see Changing Plot Defaults on page 13-17.

Adding a Time Stamp

A time stamp can be added to a plot to mark the date and time that the plot was created. The time stamp can include any combination of:

- Date
- Time
- Version
- RunID
- Username

To add a time stamp to a plot:

1. Display the plot.
2. From the Edit menu, click Insert Time Stamp.

The time stamp is simply text. To modify the time stamp, use the same instructions for modifying text.

You can also change the default time stamp for plots. For information on changing plot defaults, see Changing Plot Defaults on page 13-17.

Working with Plots

This section describes working with plots, including:

Updating Plots When Results Change

If you leave a Plot window open when you rerun a simulation, by default Aspen Plus does not redraw the plot using data from the new run.

To have a plot updated when results change:

1. Display the plot that you want to modify.
2. From the Edit menu, click Live Plot.

This option can also be selected in the Plot Wizard.

Adding Data to Plots

You can add additional curves to existing plots.

To add data:

1. Display the sheet that contains the data you want to add to an existing plot.
2. Select the dependent and independent variables.

   The selected data needs to have the same x-axis variable as the existing plot. For example, if the existing plot is temperature vs. stage number, the data selected needs to be something vs. stage number.
3. From the Plot menu, click Add New Curve.
4. In the Plot Window List dialog box, click the Plot where you want to add the new data.
5. Click OK.

   The new curve is added to the plot.

Comparing Runs Using Plots

You can use the Add New Curve feature to compare the results from different runs in a single plot.

1. After the first simulation, create the plot.
2. From the Plot menu, ensure that the Animate Plot option is not checked.
3. Change the input specifications and re-run the simulation.
4. Display the results sheet containing the data you want to compare against the first run. Select the same independent and dependent variables as in the first plot.
5. From the Plot menu, click Add New Curve.
6. In the Plot Window List dialog box, click the Plot where you want to add the new data.
7. Click OK.

   The new curve will be added to the plot.

Deleting Data Points and Curves from Plots

From an existing plot, you can delete:

- Selected data points
- An entire curve

After you delete data points from a plot, Aspen Plus redraws the curve automatically.

Note You cannot recover deleted data points. You must regenerate the plot if you want to see them again.

To delete selected data points from a plot:

1. Display the plot.
2. Hold down the left mouse button and drag the cursor to form a rectangular outline around the data points that you want to delete.
3. Click the right mouse button.
4. From the menu that appears, click Delete Points.

   Note You cannot recover deleted data points.

To delete an entire curve:

1. Display the plot.
2. Click the right mouse button.
3. From the popup menu, point to Modify, then click Hide Variable.
4. Select a variable and use the Hide and Show arrow buttons to move the desired variables from the Shown Variables list to the Hidden Variables list.

   Hidden curves can later be revealed using these same steps.

Displaying a Different Range of Data on a Plot

Use the zoom commands to display a different range of data on a plot:

This zoom option	Zooms
Zoom Auto	In by an automatic amount
Zoom Out	Out by an automatic amount
Zoom Full	To the full plot

For example, to zoom in on a specific range of data:

1. Display the plot.

2. Select the region of interest on the plot. To do this, hold down the left mouse button and drag the cursor to form a rectangle outline.
3. Click the right mouse button in this region and from the menu that appears, click Zoom In to display the region you selected.
4. To display the entire plot again, click the right mouse button in the plot and from the popup menu, click Zoom Full.

Changing Plot Defaults

To change the defaults used to generate a plot:

1. From the Tools menu, click Options.
2. From the Plots tab, click the defaults that you want to change.
3. Click the Title, Axis label, Axis scale, or Annotation buttons to modify the default font for the different types of text on a plot.
4. Use the lists to select the Grid Style and the Line Style used for new plots.
5. Use the Marker Size box to specify the size of data markers in plots.
6. Check the Show legend and/or Show Time Stamp boxes to display these elements by default on a new plot. The components of the time stamp can also be selected in this manner.

Printing a Plot

You can print a selected plot. To do this:

1. Display the plot that you want to print.
2. From the File menu, click Print.

For more information on printing, see Chapter 14.

14 Annotating Process Flowsheets

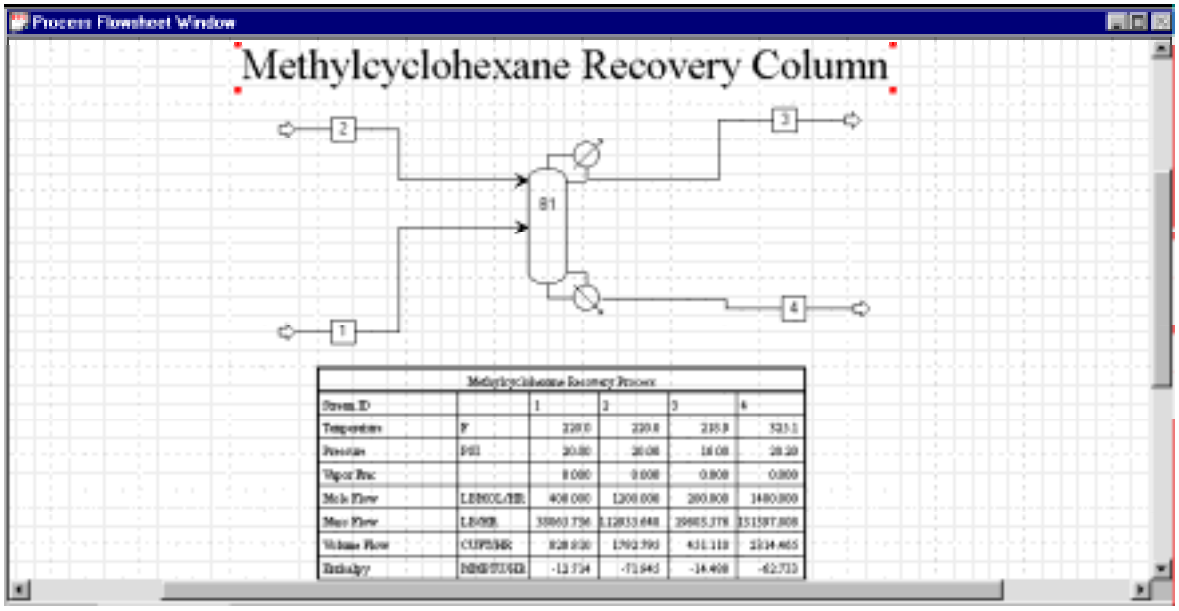
This chapter describes how you can annotate your flowsheets, including:

- Adding annotations
- Displaying global data
- Using PFD mode
- Printing

Adding Annotations

Additional text, graphics, and tables can be added to your flowsheets.

For example, this illustration shows annotation turned on to show a title and a table of stream results.



Adding Stream Tables

You can add stream tables to your flowsheets to display stream properties in a birdcage format.

To generate a stream table in your flowsheet:

1. Ensure that the flowsheet has results available. If results are not available, run the simulation.
2. From the View menu, ensure Annotation is selected.
3. Display the Results Summary Streams sheet. To do this, in the left pane of the Data Browser, click Results Summary, then Streams.

   Results for all of the streams are displayed. For more information see Chapter 12.

   If you only want selected streams to be displayed:

   - In the Display box, select Streams instead of All Streams.
   - Then select the desired stream from the list at the top cell of each column.
4. In the Format box, select the format you want. The format controls how Aspen Plus displays results. Options include order, labels, units, and precision. (See Chapters 12 and 36)

   The different formats are created using Stream Summary Format Files (*.tff files). All of the files with this extension in the system directory or in the working directory will appear in the Format list.
5. Click the Stream Table button.

Aspen Plus adds the stream table to your drawing.

The table is scaled for printing so if you cannot read its contents on screen, you can zoom in on it, or resize it.

6. Move the table to the position you want, using the keyboard or mouse.
7. You can attach the table to a block or stream. From the Table popup menu, click Attach.
8. To arrange the table in multiple rows of streams, from the Table popup menu, click Stack Table.

Resizing Stream Tables

You can resize stream tables by changing the font size. To do this:

1. Click on the stream table to select it.
2. On the Draw toolbar, change the font size.

   The stream table resizes accordingly.

Adding Graphics Objects

To add lines, circles, or boxes to a flowsheet:

1. From the View menu, ensure Annotation is selected.
2. Ensure the Draw toolbar is displayed. Click here for more information.

   To do this, from the View menu, click Toolbar and ensure Draw is selected.
3. From the Draw toolbar, select the drawing tool that you want, and the line style and fill color that you want.
4. Move the cursor to where you want to place the object.
5. Hold down the mouse button until the cursor changes to the resize shape (+).
6. Drag the cursor to create the object in the size you want, then release the mouse button.
7. To fill in the graphics object, select the object and check fill on the object's popup menu.

You can change the attributes of an object after you place it. Select the object, then select the line style or fill color from the Draw toolbar.

Use the mouse or keyboard to move and resize graphics objects. You can attach the graphics object to a block or stream by clicking the block or stream with the right mouse button and from the popup menu that appears, clicking Attach.

It is helpful to show the grid and use grid options when placing, moving, and resizing graphics objects. For more information see Aligning Objects in Flowsheets on page 14-12. For information on how to use and customize the Grid and Scale options, see Chapters 4 and 16.

Adding Text Objects

To add text annotations to a flowsheet:

1. On the View menu, ensure Annotation is selected.
2. Ensure the Draw toolbar is displayed. Click here for changing which toolbars are displayed.

   To do this, from the View menu, click Toolbar and ensure Draw is selected.
3. From the Draw toolbar, click the text button  .
4. Move the cursor to where you want to place the text and click the mouse button.
5. Type the text.

   Use the mouse or keyboard to move and resize text you have placed.

   You can also attach the object to a block or stream. To do this, click the block or stream with the right mouse button and from the popup menu that appears, click Attach.

It is helpful to show the grid and use grid options when placing, moving, and resizing text. For more information see Aligning Objects in Flowsheets on page 14-12. For information on how to use and customize the Grid and Scale options, see Chapters 4 and 16.

Specifying Text Attributes

You can change the appearance of text objects after you place them in your flowsheet by selecting the text object then using the Draw toolbar to specify the attributes.

To specify the default text attributes for all subsequent text that you add:

1. Ensure no text objects are selected in the drawing.
2. In the Draw toolbar, specify the attributes you want.

Editing Text Objects

In a flowsheet, you can edit a text object.

To edit a text string:

1. Select the text string and click the right mouse button.
2. From the popup menu that appears, click Edit.

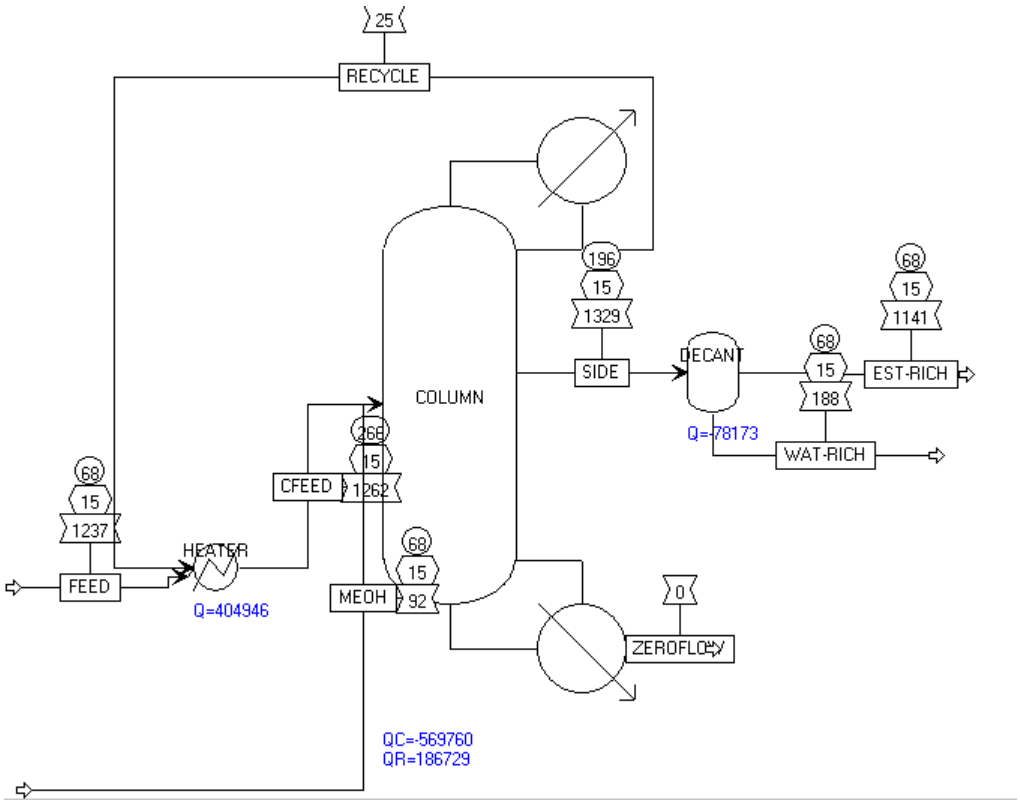
About Global Data

Global data consists of simulation results for each stream, and for each block that calculates duty or power.

You can display the following global data directly on a flowsheet:

This data	Is displayed
Stream temperature, pressure, flow rate	In symbols attached to stream IDs
Heat stream duty	In symbols attached to stream IDs
Work stream power	In symbols attached to stream IDs
Block heat duty and power	Next to the block icon

This example shows a process flowsheet window where global data is turned on to show temperature, pressure, and flow rate for each stream:



Displaying Global Data

To display global data in a flowsheet:

1. From the View menu, ensure Global data is selected.
2. Ensure that the flowsheet has results available. If results are not available, run the simulation.
3. From the Tools menu, click Options.
4. Click the Results View tab.
5. Select a units set for the data from the list.
6. Select the results you want to display.

   For each result, specify a numerical format.

   The recommended format is %10.2f. This format prints values with two digits to the right of the decimal, if there is room. If the number is greater than 9,999,999, Aspen Plus eliminates the fractional digits, then spills over the field range to the left.

Other common formats used in stream tables are:

Stream table format	Prints
%10.0f	Whole numbers, with no decimal digits or exponents
%10.nf	Numbers without exponents and with n digits to the right of the decimal point, if there is room. Decimal points line up, unless decimal digits have been eliminated in some numbers.
%10.nE	Numbers in exponential notation, with n+1 significant digits

7. Click OK to close the dialog box and display the data.

   A legend box shows the global data symbols and units. You can move and resize the legend in the same way that you move and resize blocks.

About PFD Mode

Aspen Plus has a special Process Flow Diagram (PFD) mode that enables you to create customized diagrams from your simulation results. In this mode, you can add or delete unit operation icons to the flowsheet for graphical purposes only.

Using PFD mode means that you can change flowsheet connectivity to match that of your plant.

To use the PFD mode:

➤ Turn PFD mode on and off from the View menu.

The default is PFD Mode turned off.

Using PFD Mode to Change Flowsheet Connectivity

In the simulation flowsheet, you may need to use more than one unit operation block to model a single piece of equipment in a plant. For example, a reactor with a liquid product and a vent may need to be modeled using a RStoic reactor and a Flash2 block. In the report, only one unit operation icon is needed to represent the unit in the plant.

Alternatively, some pieces of equipment may not need to be explicitly modeled in the simulation flowsheet. For example, pumps are frequently not modeled in the simulation flowsheet; the pressure change can be neglected or included in another unit operation block.

When PFD mode is on, you can:

- Add blocks and streams that are not in the simulation flowsheet
- Delete blocks and streams that are in the simulation flowsheet

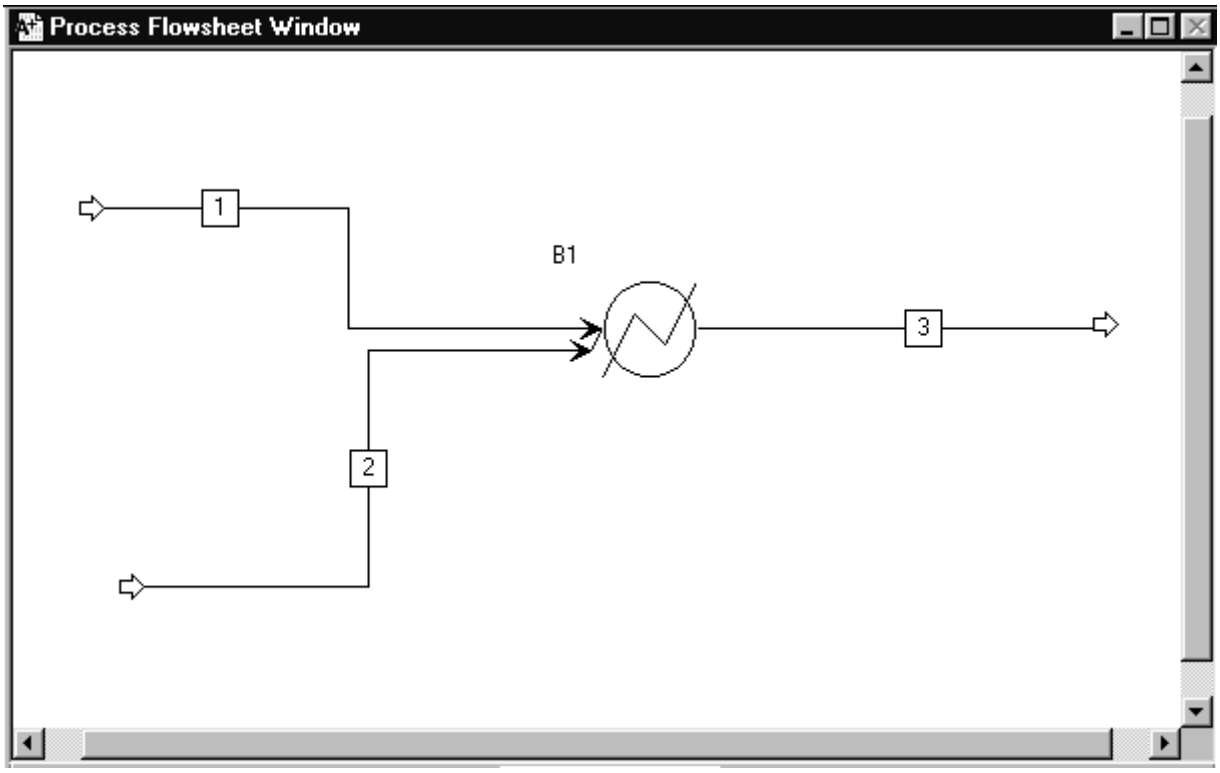
In summary:

Have PFD mode	When you
Off	Create a simulation flowsheet (default)
On	Prepare customized PFD-style drawings for reports

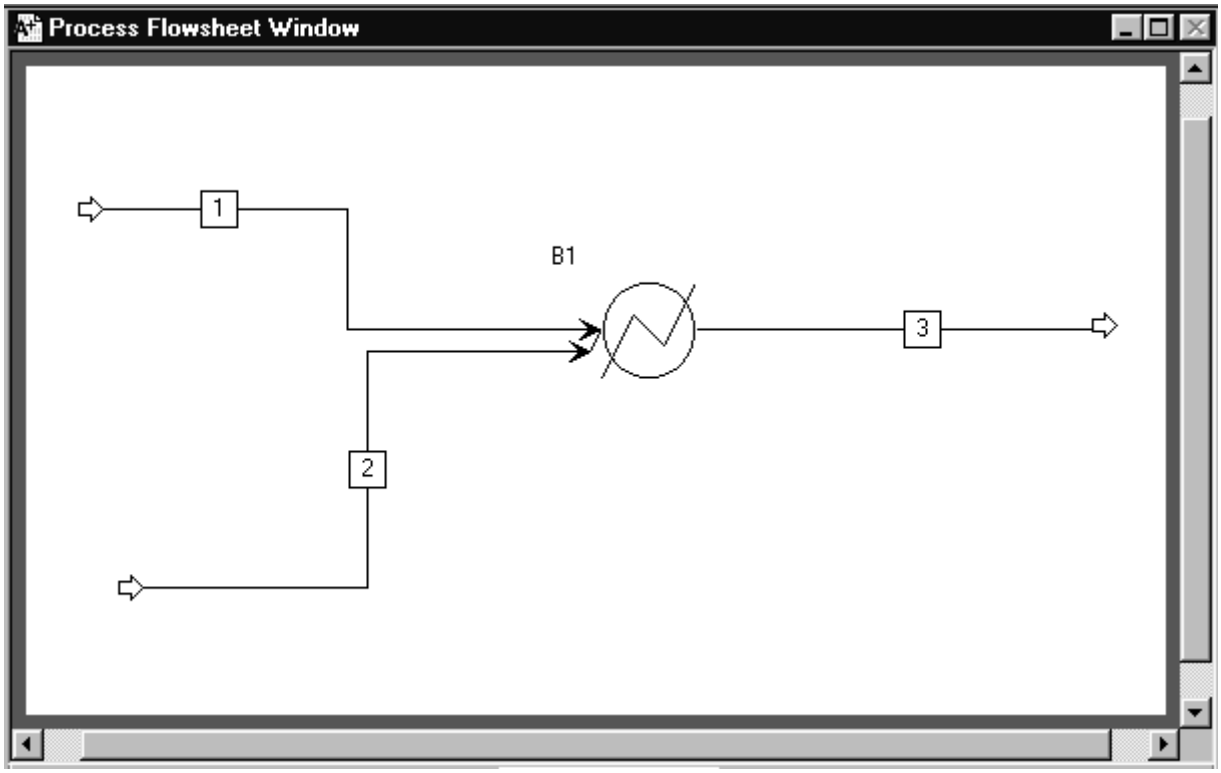
Example of Aspen Plus in Simulation Mode and PFD Mode

When the PFD mode is on, PFD mode is shown on the status bar and a aqua border is displayed at the edge of the Process Flowsheet Window.

Simulation Mode:



PFD mode:



Creating a Process Flow Diagram

To create a process flow diagram:

1. Display the simulation flowsheet.
2. From the View menu, ensure PFD mode is checked.

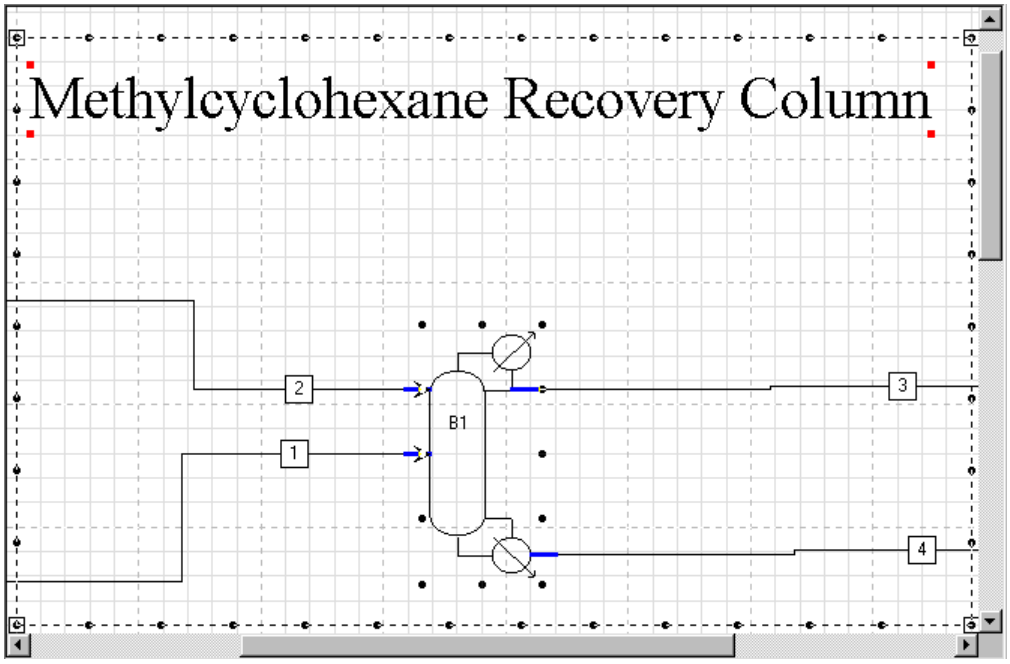
   You are now in PFD mode. Aspen Plus displays a copy of your simulation flowsheet.
3. Modify the drawing, as described in subsequent sections of this chapter.
4. To exit PFD mode, from the View menu, clear the PFD mode checkbox.

Important PFD-style drawing is completely separate from the graphical simulation flowsheet. You must return to simulation mode if you want to make a change to the simulation flowsheet.

Grouping Objects

You can create temporary or permanent groups of text and graphics objects in your flowsheet.

example, this diagram shows a temporary group that includes the text "Methylcyclohexane Recovery Column" and the Unit Operation Icon for the column:



You can select a region containing both the objects and flowsheet blocks and streams. You can move the selected text, graphics, and flowsheet objects as a unit. But you must perform all other operations separately for the different groups in the region.

When you select a temporary group, you can move, resize, or change attributes of all objects in the group together.

A permanent group becomes a single object in the drawing. You can select, move, resize, rotate, or change the attributes of all objects in the group together. You can attach the entire group to a flowsheet block or stream. For more information, see Attaching Objects to the Flowsheet on page 14-13.

Creating Temporary Groups

To create a temporary group in your flowsheet:

1. Select a region that contains text or graphics objects by using the mouse to draw a box around the region.
2. You can add or remove objects by holding down Ctrl and clicking the mouse.
3. Work with the selected group to perform the operations you want. For more information see Working with Temporary Groups on page 14-11.
4. To deselect the group, move the mouse away from the group and click.

Working with Temporary Groups

After creating a temporary group, you can perform these operations:

To do this	Use the	And
Move the group	Keyboard or mouse	Move the group as if it were a single object.
Resize the group	Resize button or + and - keys	Drag the mouse or hold down the key until the group is the size you want
Change attributes	Draw toolbar	Select the attribute you want.
Zoom in or print	Popup menu. Click the right mouse button within the region, but outside the group select buttons.	Select Zoom In or Print.
Use other group commands	Popup menu. Click the right mouse button on the group.	Select a command.

Creating Permanent Groups

To create a permanent group:

1. Select a temporary group.
2. Click with the right mouse button on an object in the group.
3. From the Group popup menu that appears, click Group.

   You can attach a permanent group to a flowsheet block or stream.

Making Permanent Groups into Temporary Groups

To convert a permanent group to a temporary group:

1. Click the right mouse button on the group

2. From the Group popup menu that appears, click Ungroup.

Aligning Objects in Flowsheets

If the Snap to Grid option is on, any text or graphics objects that you add or move align to a grid.

To display the grid:

1. From the Tools menu, click Options.
2. Click Grid/Scale.
3. Check Show Grid to see the grid on the screen.

You may need to position or size objects more precisely than the default grid allows.

You can turn off the Snap to Grid option, reduce the grid size and display a ruler.

- Turn off the Snap to Grid option
- Reduce the grid size

You can also use the Process Flowsheet toolbar to perform all these operations quickly.

To turn off the Snap to Grid option:

1. From the Tools menu, click Options.
2. Click the Grid/Scale tab.
3. Clear the Snap to Grid checkbox.

To change the grid size:

1. From the Tools menu, click Options.
2. Click the Grid/Scale tab.
3. Select the Grid Size from the list.

You can display a ruler to help you see where you are within the overall drawing grid:

1. From the Tools menu, click Options.
2. Click the Grid/Scale tab.
3. Check Show Scale to turn it on.

When precisely aligning text and graphics, it is helpful to zoom in on the area of the flowsheet where you are working.

Attaching Objects to the Flowsheet

You can attach stream tables, permanent groups, and OLE objects to flowsheet blocks or stream IDs. Attached objects move with the parent block or stream ID. For example, text annotation attached to a block maintains its position relative to the block, no matter where you move the block in a drawing.

To attach an object to a flowsheet:

1. Click the object to select it.
2. Click the right mouse button on the object.
3. From the popup menu that appears, click Attach.

   The mouse changes to the connect pointer.
4. Click the block or stream to which you want the object connected.
5. Move the object where you want it, relative to the parent block or stream ID.

When you select an attached object, small boxes indicate the parent block or stream.

To unattach an object:

➤ From the object's popup menu, deselect Attach.

Printing

This section contains information on:

- Specifying your print settings in the Page Setup dialog box
- Viewing the page layout and adjusting the page breaks

You can print the following in Aspen Plus:

- The entire flowsheet
- A section of a flowsheet
- Plots
- Online Documentation and Help

Tip To print Aspen Plus forms, copy and paste the information to Microsoft Excel, then print.

Using Page Setup

Use Page Setup to control the appearance of printed sheets, paper size, including margins, orientation, and other printing options.

Aspen Plus uses the Number of Pages setting only when you print an entire drawing or flowsheet section. Aspen Plus superimposes the drawing on a page layout. The layout is defined by:

- Number of vertical and horizontal pages
- Page orientation
- Paper size

You can use Page Break Preview on the View menu to see where the page breaks are located on the drawing.

Aspen Plus scales drawings proportionally to fill the page in the limiting direction (horizontal or vertical), within built-in margins. It does not distort the drawing to fill the page in both directions.

Specify your settings for printing the flowsheet window on the Page Setup dialog box:

↗ From the File menu, click Page Setup.

Viewing Page Breaks

You can view the page breaks in order to visualize the layout and adjust what is going to be printed. You should avoid printing drawings with icons or IDs spanning page boundaries.

Adjust the position of the drawing on the page by:

- Repositioning the flowsheet objects on the individual pages
- Moving and resizing the page layout frame

You can change the page layout at any time by changing the settings on Page Setup. Aspen Plus will redraw the page breaks.

To view the page layout:

1. From the View menu, click Page Break Preview.
2. Complete the Page Setup dialog box or accept the defaults if this sheet has not been viewed previously.

   In the Page Setup dialog box, you can specify the number or horizontal and vertical pages, the paper size and source, the paper orientation (portrait or landscape), and the margins.

3. When the flowsheet is superimposed on the current page layout, you can select the borders to move the location of the pages, and you can select a corner to change the size of the pages relative to the flowsheet.

   Note All the pages must remain equally sized.

4. You can also move elements of the flowsheet such as the unit operation icons, tables, and annotation to a desired location. In this way, you can determine what is present in the print area.

   Hint It is often helpful to select Zoom Full from the View menu in order to view the entire Flowsheet before adjusting the page breaks.

Printing a Flowsheet

To print a flowsheet:

1. Click in the Process Flowsheet Window to make it active.
2. Click the Printer button on the Standard toolbar.

   – or –

   From the File menu, select Print.
3. Choose the printer and desired settings in the Print dialog box.
4. Click OK.

Printing a Section of Flowsheet

To print a section of flowsheet:

1. From the Flowsheet menu, click Flowsheet Sections.
2. Choose the flowsheet section you want to print and click OK.
3. From the View menu, click Current Section Only.
4. Click the Printer button on the toolbar.

   – or –

   From the File menu, select Print.
5. Choose the printer and desired settings in the Print dialog box.
6. Click OK.

Displaying and Printing Attached Objects with Flowsheet Sections

In a flowsheet divided into sections, when the View only current section option is on in the Section Object Manager, attached objects display and print with the section they are attached to.

For example, you can generate a stream table consisting of all the streams in a section and attach it to a block in the section. If you print the section, the stream table prints with it. Unattached annotation objects or OLD objects display and print with all sections. For more information on flowsheet sections, see Chapter 4.

Printing Large Flowsheets

For large flowsheets, it is often necessary to print the flowsheet on multiple pages. You may also want to only print one flowsheet section at a time.

To print on multiple pages:

1. From the File menu, click Page Setup.
2. Specify the desired number of horizontal and vertical pages.
3. From the View menu, click Page Break Preview.
4. Select the page borders to move the location of the pages, or select a corner to change the size of the pages relative to the flowsheet.

   Note All of the pages must remain equally sized.
5. You can also move elements of the flowsheet such as the unit operation icons, tables, and annotation and arrange them to fit on a desired page.

15 Managing Your Files

This chapter describes how to manage the files you create when running Aspen Plus including:

- File formats used during Aspen Plus runs
- Saving Aspen Plus document files
- Exporting Aspen Plus files
- Importing Aspen Plus files
- Saving an Aspen Plus run
- Managing files in a client-server environment

File Formats in Aspen Plus

These are the major types of files used in Aspen Plus:

File Type	Extension	Format†	Description
Document	*.apw	Binary	Quick restart file containing simulation input and results and immediate convergence information
Backup	*.bkp	ASCII	Archive file containing simulation input and results
Template	*.apt	ASCII	Template containing default inputs
Input	*.inp	Text	Simulation input
Run Message	*.cpm	Text	Calculation history shown in the Control Panel
History	*.his	Text	Detailed calculation history and diagnostic messages
Summary	*.sum	ASCII	Simulation results
Problem Definition	*.appdf	Binary	Binary file containing arrays and intermediate convergence information used in the simulation calculations
Report	*.rep	Text	Simulation report

† *In this context a "text" file is one that you can read using a standard editor such as Notepad®. A binary file cannot be read by the user. An ASCII file can be opened in an editor, but is formatted to be read by a program, not a person. ASCII files are portable across different hardware platforms.*

Document Files (*.apw)

Aspen Plus document files contain all input specifications, simulation results, and intermediate convergence information. If you save a run as a Document file before you exit from Aspen Plus, the next time you open the run it is in exactly the same state as when you saved it. If you reopen a run saved as a Document file, Aspen Plus restarts the calculations using the previous results.

Document files can be opened in the Aspen Plus User Interface and saved.

Disadvantages

Document files (.apw) are not compatible across different versions of Aspen Plus.

Advantages

For longer simulations, Document files are much quicker to load into and save from the Aspen Plus User Interface.

Because Document files contain intermediate convergence information, the run can be started exactly where it was saved. Intermediate results are especially useful when you save a file while in the process of trying to converge a large flowsheet.

Backup Files (*.bkp)

Aspen Plus Backup files contain a compact version of your Aspen Plus run. They occupy much less disk space than files saved in Document format, and are thus preferable for long-term storage.

Backup files contain all input specifications and simulation results, but no intermediate convergence information. If you reopen a converged run stored as a backup file and rerun the simulation, Aspen Plus:

- Reinitializes the streams and blocks
- Reconverges the entire simulation

Backup files are ASCII files. You can use them to transfer runs between:

- Computers
- Versions of Aspen Plus

The advantage of the Backup (.bkp) files over Document (.apw) files is that the Backup files are upwardly compatible through different versions of Aspen Plus and are portable. For example, they can easily be emailed.

Backup files can be opened and saved in Aspen Plus. They can also be imported into a current run, and partial or complete flowsheets can be exported. For more information, see Exporting Aspen Plus File on page 15-8.

You can import runs saved in Backup format into your current run. Aspen Plus merges the information and specifications contained in the backup file with your current run.

For example, you can have two sections of a flowsheet stored in separate backup files. You can import these two backup files into a single run, merging the two flowsheet sections.

For information on inserts (partial backup files that you can import at any time), see Chapter 34.

Maintaining Upward Compatibility

When importing a backup file, you can control compatibility between Aspen Plus versions.

The Upward Compatibility dialog box appears when you open a backup file that was created with the Aspen Plus simulation engine, or with a previous version of Aspen Plus.

New features in Aspen Plus Version 10 may mean your results differ from those of previous versions. To maintain upward compatibility and obtain the same results as your previous version of Aspen Plus, ignore the new features of Version 10. To do this:

In the Upward Compatibility dialog box, select Maintain Complete Upward Compatibility.

To use the new features of Version 10:

In the Upward Compatibility dialog box, select Use the Following New Features, and check the features you want from:

- New pure component databanks
- New property methods
- New built-in binary parameters
- New ADA/PCS procedures
- Calculated molecular weight obtained from formula
- Checking of user-specified sequence

Note If you are opening a file created by Version 9 of the Aspen Plus user interface, you will get only the option of using the new pure component databank, PURE10.

Template Files (*.apt)

You can select a Template when creating a new run. Templates set defaults for some or all of the following:

- Units of measurement
- Property sets for reporting stream properties
- Composition basis for stream reporting
- Stream report format
- Global flow basis for input specifications
- Setting for Free-Water option
- Selection for Stream-Class
- Property option set
- Required components (such as water)
- Other application-specific defaults
-

For detailed information on the built-in template and creating templates, see Chapter 2.

Input Files (*.inp)

Aspen Plus input files are compact summaries of the specifications for a flowsheet simulation. An input file can include graphical information about the layout of the unit operation blocks and streams in the Process Flowsheet Window.

An input file can:

- Be used as the input file for a stand-alone Aspen Plus engine run
- Provide a compact summary of the input specifications for a simulation (for example, to be included in a report)
- Provide the documentation of record for a simulation study (for example, as part of the archives for a design project)
- Help expert users diagnose problems

You can generate an Aspen Plus input file from your simulation specifications at any time. To save an input file, you must export it from the Aspen Plus user interface.

The input file can be run directly by the simulation engine. Click here for details.For more information on how to run an input file using the simulation engine, see Chapter 11.

Import the backup file as described in Importing Aspen Plus File on page 15-8.

Report Files (*.rep)

Aspen Plus Report files document all of the input data and defaults used in an Aspen Plus run, as well as the results of the simulation. These are text files that can be read by the user.

Report files must be exported from the simulation to be saved. Report files cannot be opened in the Aspen Plus User Interface.

If applicable, the DFMS input file (*.dfm), the Prop-Data file (*.prd) and the Project file (*.prj) are exported along with the report file.

Summary Files (*.sum)

Aspen Plus Summary files contain all the results from the simulation that are displayed in the Aspen Plus user interface. Summary files are ASCII format files used to load the results into the user interface. Summary files can also be used by other programs to retrieve the results of the simulation.

Summary files must be exported from the simulation to be saved. For more information, see Exporting Aspen Plus File on page 15-8. Summary files are automatically generated when running the Aspen Plus simulation engine standalone. The summary file generated is called *runid*.sum.

The results included in summary files can be imported in the Aspen Plus User Interface. For more information, see Importing Aspen Plus File on page 15-8.

Run Messages Files (*.cpm)

Aspen Plus Run Messages files are text files that include the error, warning, and diagnostic messages from the run. These are the messages displayed on the Control Panel during a run. The number of messages and the detail can be controlled globally on the Setup Specifications Diagnostics sheet. You can also control the messages localy for each block on the block BlockOptions Diagnostics sheet.

Run Messages files are similar to history files (*.his). The diagnostic level for history files and the control panel can be adjusted independently. If you need a high level of diagnostics, print to the history file (not to the control panel). This prevents any performance degradation that might result from lengthy diagnostics on the screen.

Run Messages files must be exported from the simulation to be saved.

History Files (*.his)

The History file is a text file that includes an echo of the input summary and the error, warning, and diagnostic messages from the run. The number of messages and the detail can be controlled globally on the Setup Specifications Diagnostics sheet. You can also control the messages locally for each block on the block BlockOptions Diagnostics sheet.

When you select History from the View menu, the Aspen Plus history file is copied from the host computer to your local computer. Aspen Plus executes your file editor to view the history file.

A history file cannot be saved or exported from the Aspen Plus User Interface. Save the file using History from the View menu. A history file is saved automatically when you save a run as a Document file.

The history file is similar to the Run Messages file. The diagnostic levels for the history file and the control panel can be adjusted independently. If you need a high level of diagnostics, print to the history file (not to the control panel). This prevents any performance degradation that might result from lengthy diagnostics on the screen.

Opening Aspen Plus Files

You can open an existing Aspen Plus file from within Aspen Plus.

1. From the File menu, click Open.
2. In the Open dialog box, select the file type from the Files of Type list.
3. Enter a filename or select a file from the available list, then click Open.
4. The message “Do you wish to close the current run before opening new run?”, appears. Click No for the new simulation to be opened in a separate window. Click Yes to close the current run.

   Tip To speed up your search for files or directories, in the Open dialog-box. click the Look in Favorites button to display a list of pre-selected directories. Use the Add to Favorites button to place frequently used directories into this list.

Using the Favorites List

By default, the Favorites list contains 5 directories that are provided with Aspen Plus. The files in these directories are designed to assist you in creating a suitable simulation model in Aspen Plus.

This table shows the directories:

Directory	Description
Assay Libraries	Petroleum crude assays compiled from literature for different regions of the world and selected crude assays from the Phillips Petroleum Crude Assay Library
Applications	Application examples of real world problems covering gas processing, petroleum refining, chemicals, pharmaceuticals, and metals processing industries
Data Packages	Special property data packages for industrially important systems
Examples	Selected examples
Electrolyte Inserts	Electrolyte data packages for many industrially important systems

Saving a Run

To save a file in Aspen Plus:

1. From the File menu, click Save As.
2. In the Save As dialog box, select the appropriate file type from the Save as Type list.
3. Enter a filename. The file can be saved in any directory.
4. Click Save.

You can save these types of files:

File Type	Extension	Description
Document	.apw	Quick restart file containing simulation input and results and intermediate convergence information
Backup	.bkp	Archive file containing simulation input and results
Template	.apt	Template containing default inputs

Exporting Aspen Plus Files

To generate and export an Aspen Plus file:

1. From the File menu, click Export.
2. In the Export dialog box, select the appropriate file type from the Save as Type list.
3. Enter a filename. The file can be saved in any directory.
4. Click Save.

You can export the following types of Aspen Plus files:

File Type	Extension	Format	Description
Backup	.bkp	ASCII	Archive containing simulation input and results
Report	.rep	Text	Report file
Summary	.sum	ASCII	Simulation results
Input	.inp	Text	Simulation input information without graphics
Input File with Graphics	.inp	Text	Simulation input and graphical information
Run Messages	.cpm	Text	Calculation history
Flow Driven Dynamic Simulation	.spf .inp	Text	Aspen Dynamics input and Aspen Plus input
Pressure Driven Dynamic Simulation	.spe .inp	Text	Aspen Dynamics input and Aspen Plus input

Importing Aspen Plus Files

To import an Aspen Plus file:

1. From the File menu, click Import.
2. In the Import dialog box, select the file type from the Files of Type list
3. Enter a filename. The file can be saved in any directory.
4. Click Open.
5. If the Resolve ID Conflicts dialog box appears, there are objects that have the same ID as objects in the current run. For information about using the Resolve ID Conflicts dialog box, see Chapter 38.

Tip To speed up your search for files or directories, in the Open dialog-box. click the Look in Favorites button to display a list of pre-selected directories. Use the Add to Favorites button to place frequently used directories into this list.

You can import the following types of files:

File Type	Extension	Format	Description
Backup	*.bkp	ASCII	Archive containing simulation input and results
Template	*.apt	ASCII	ASCII file used as a template
IK-Cape	.ikc	ASCII	IK-Cape neutral file for physical property information
Summary	*.sum	ASCII	Simulation results

Deciding How to Store a Simulation Problem Definition

You can save an Aspen Plus simulation in the following threeways:

- Save the Aspen Plus Document file
- Save the Aspen Plus Backup file
- Export the file as an Input file

This table summarizes the characteristics of the file formats used to store the simulation problem:

Characteristic	Document	Backup	Input
Simulation Definition (input specifications)	✓	✓	✓
Intermediate Convergence Information	✓		
Results	✓	✓	
Graphics	✓	✓	✓
User Readable			✓
ASCII Format		✓	✓
Readable by Aspen Plus User Interface	✓	✓	✓

Managing Files in a Client-Server Environment

You can run the Aspen Plus user interface and the simulation engine:

- On the same computer
- On different computers in your network

Usually, you do not need to be aware of how or where Aspen Plus is installed. However, you should be aware of some file management issues, described in the following sections.

The local computer is where the Aspen Plus user interface is running. The host computer is where the Aspen Plus simulation engine is running.

Specifying the Working Directory on the Host Computer

If you have not specified a working directory, files created by the Aspen Plus simulation engine are stored in your default login directory on the host computer. To specify the working directory where the simulation engine should execute:

From the Run menu, click Connect to Engine.

Saving Files

When you save a run as an Aspen Plus Document (.apw) file using Save or Save As from the File menu, Aspen Plus creates these files in the following locations:

File	Location
runid.apw	Local directory where you are running the user interface, or the directory specified on the Save As dialog box
runid.his	Working directory on host computer specified in the Connect to Engine dialog box
runid.appdf	Working directory on host computer specified in the Connect to Engine dialog box

View History

To copy the Aspen Plus history file from the host computer to your local computer:

From the View menu, click History.

Aspen Plus executes your file editor to view the history file.

Tip If the history file is large, copying the history file to your local computer can take a long time. In such a case, you should log onto the host computer and view the file.

Specifying the Text Editor

To specify the text editor:

1. From the Tools menu, click Options.
2. Click the Startup tab.
3. In the Text Editor box, type the name of the editor.
4. Click OK

16 Customizing Your Aspen Plus Environment

Configuration options are default settings that affect how you use Aspen Plus. For example, configuration options enable you to specify:

- Grid and scale settings
- Default Application Template file
- Which binary databanks are used as defaults

This chapter explains:

- Choosing settings for the current run
- Choosing settings for all runs
- Specifying your default options
- Customizing Application Template files

Choosing Settings for the Current Run

To change your configuration option settings for the current run:

From the	You can select
View menu	Any command
Tools menu	Options
Window menu	Any command

Customizing Settings for All Runs

To create a custom environment for subsequent Aspen Plus runs:

1. Open a blank run.
2. Customize the settings, then exit.

   You do not need to save the blank run.

   Your customized settings are saved in the Windows registry and are used for all subsequent runs. If you modify any settings, the new settings are used in subsequent runs.

   Note Some settings are saved with the simulation. If a setting that is saved with a simulation differs from the setting in the registry, the setting that is saved with the simulation will be used for that simulation; however, subsequent simulations will use the setting that is in the registry.

Choosing View Options

You can change which elements are visible by using the options on the View menu. Display or hide elements, depending upon what you need at any given time.

These options are available from the View menu:

Click this option	To
Toolbar	Select the toolbars that are displayed
Status Bar	Select if the status bar on the main window is displayed
Model Library	Select if the Model Library is displayed
Control Panel	Select if the Control Panel is displayed
Zoom In	Magnify a portion of the drawing on the screen. If a Group or Region has been selected, the selected region will be expanded to fill the screen. When you zoom in on a selected region, the portion of the drawing displayed may not be exactly what you selected, since proportional vertical/horizontal scaling is maintained at all times.
Zoom Out	Shrink the drawing on the screen in order to show more of the drawing or to make room for more blocks or symbols. As you shrink the drawing, text and some symbols will disappear from the screen due to the screen resolution. These objects are not deleted, they reappear when you zoom in, and print.
Zoom Full	Display the entire drawing as large as possible in the workspace
Center View	Display the selected object in the center of the screen

Continued

Click this option	To
Pan	Choose a region of the flowsheet to display at the current zoom level
Bookmarks	Create bookmark views or got to a bookmark
Page Break Preview	Select if the page breaks are displayed in the Process Flowsheet window For more information see Chapter 14.
Reset Page Breaks	Reset page breaks you have defined
Current Section Only	Select if only the current flowsheet section is displayed For more information on using flowsheet sections see Chapter 4.
PFD Mode	Select whether PFD mode is on or off.
Reset PFD	Delete the current PFD mode drawing and create a new one
Global Data	Select if global data is displayed for each stream. See Results View Options for information about how to customize the global data.
Annotation	Select if text annotation on the Process Flowsheet window is displayed
OLE Objects	Select if OLE objects are displayed For more information, see Chapter 38.
Input Summary	View the input summary For more information about the input file, see Chapter 15.
History	View the history file For more information about the history file, see Chapter 15.
Report	View a section of the report file For more information about the report file, see Chapter 12.

Using Toolbars

The buttons on a specific toolbars cannot be customized. However, the toolbars can be viewed, hidden, or moved to another location.

Toolbar settings are not saved with the simulation file. The toolbar configuration is saved in the registry and will be used for all subsequent files that are opened in Aspen Plus.

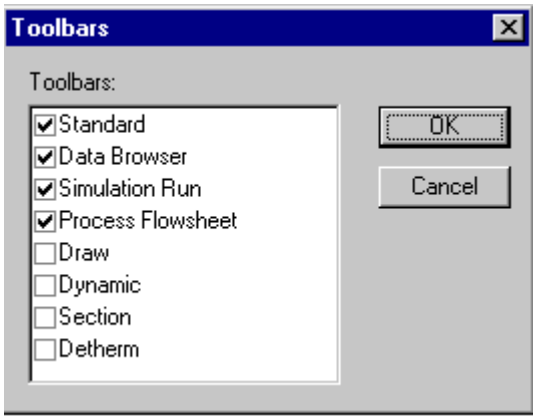
These toolbars are available:

Toolbar	Buttons
Standard	Standard Windows buttons used for basic operations New, Open, Save, Cut, Print, Print Preview, Copy, Paste, Help
Data Browser	Buttons used to display the next required step, the Data Browser, or one of its various elements
Simulation Run	Buttons used to control the execution of the simulation
Process Flowsheet (PFS)	Buttons used to manipulate the unit operation, graphical or text objects located in the process flowsheet
Draw	Buttons used to add or modify graphical or text objects
Dynamic	Buttons used for dynamic simulations using Aspen Dynamics
Section	Buttons used to manipulate flowsheet sections
Detherm	Buttons used for Detherm application

Viewing Toolbars

You can choose which toolbars are shown in the main window of Aspen Plus. To do this:

1. From the View menu, click Toolbar.
2. Select the check box of each toolbar you want to view.



The toolbars that are checked are those that appear by default.

Moving Toolbars

Toolbars can be positioned elsewhere in the window. To do this:

1. Click and hold down the mouse button on the edge of the toolbar you wish to move.

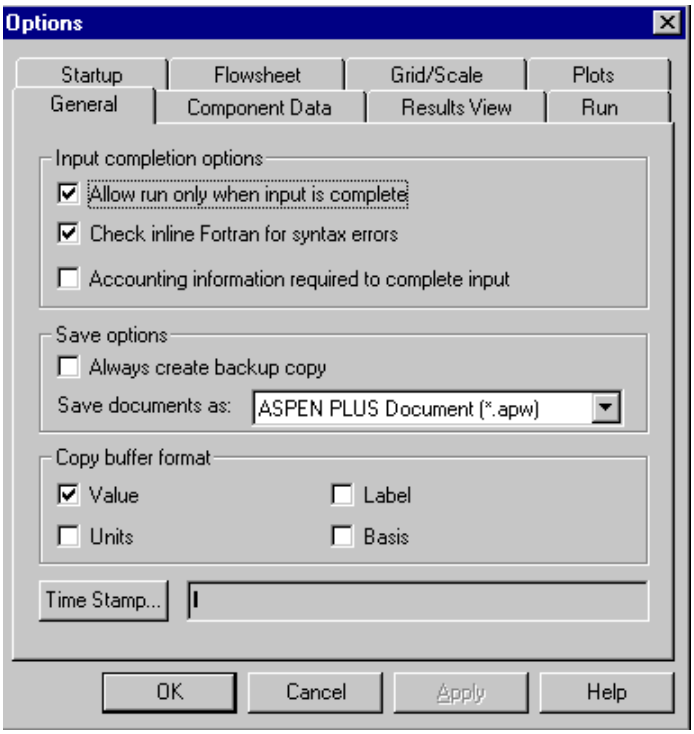
2. Drag the toolbar to the desired location, which can be either:
   - On any edge (top, bottom, or sides) of the Aspen Plus window
   - In the center of the window

Specifying Default Options

There are various options you can set as defaults. To do this:

➤ From the Tools menu, click Options.

The Options dialog box appears.



This table shows which tab to use:

To	Use this tab
Specify general options such as the default method to save documents and if inline Fortran is checked for syntax errors	General
Specify the databank search order	Component Data
Select what information is included when Global Data is displayed	Results View
Control various naming, display and placement options on the process flowsheet	Flowsheet
Set and display the grid and scale on the process flowsheet window	Grid/Scale
Specify the default fonts, grid style, line style, marker size, and time stamp components used when creating plots Select if a legend and time stamp are displayed by default.	Plots
Select run options for interactive runs and specifications for a remote server	Run
Specify startup options for a new flowsheet such as Run Type, application template, and working directory	Startup

Using the General Tab

From the Tools menu, click Options, then click General. The General tab is used to specify general options related to running simulation, saving Aspen Plus documents, and making OLE links between an Aspen Plus run and another application.

The following parameters are available on the Tools Options General tab:

Use this box	To	Saved with Simulation?
Allow run only when input is complete	Allow a run only when input is complete Turning off this option allows you to initiate an interactive or batch run even if the status in the toolbar is not Required Input Complete. This option is primarily for advanced users who are familiar with keyword input language.	Yes
Check inline Fortran for syntax errors	Check inline Fortran for syntax errors When this option is checked, basic Fortran syntax error checking is done on all the Fortran and Declarations sheets. This option sometimes needs to be turned off when advanced Fortran is used.	Yes
Accounting information required to complete input	Allow a run only when accounting information has been completed. When this option is checked, you are required to specify accounting information on the Setup Specifications Accounting sheet. The accounting information includes an account number, a project ID, a project name, and a user name. This is stored for the run by the Aspen Plus Accounting System, if it is active for your installation.	No
Always create backup copy	Always create backup copy. When this option is checked, an Aspen Plus backup format file (*.bkp) is created whenever an Aspen Plus document file (*.apw) is saved. This is used as an additional backup safety mechanism. The document file (*.apw) allows you to quickly restart previously saved simulation, using a binary file. The backup file (*.bkp) stores the same run information in a condensed ASCII file.	No
Save Aspen Plus documents as	Specify the default method to save documents. Saving documents as document files (*.apw) allows you to quickly restart previously saved simulation, using a binary file. Saving as backup files (*.bkp) stores the same run information in a condensed ASCII file.	No
Copy buffer format	Specify what information is included when a cell is copied into the copy buffer. Every variable, when copied for OLE links, occurs with four attributes: Value, Units, Label, and Basis. You can set the default attributes here, or you can specify the attributes you need, from the Edit menu by clicking Copy with Format.	Yes

Using the Component Data Tab

Use the Component Data tab to:

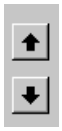
- Change the databanks search order
- Choose which databanks are searched
- Copy regression and estimation results onto Parameters forms
- Generate input language using component name or component alias

Changing Databanks Search Order

The order in which the pure and binary components databanks are searched can be changed using the Tools Options Components Data dialog box.

To change the pure and binary component databank search order:

1. From the Tools menu, click Options.
2. Click the Component Data tab.
3. In the Searched list, click the databank that you want to reorder.
4. Click the up or down arrow to reorder the databank.



The databank at the top of the list is searched first. The data found first for a component or a component pair is the data that is used in the simulation.

Pure Component Databank Search Order—This specifies which pure component databanks Aspen Plus will search and the search order for all simulations.

The order in which the databanks are listed is the order in which Aspen Plus searches for data. For a specific simulation run, you may change the list and order on the Components Specifications Databanks sheet.

Binary Databank Search Order—This specifies which binary parameter databanks Aspen Plus will search and the search order for all simulations.

The order in which the databanks are listed is the order in which Aspen Plus searches for data. These databanks contain:

- Binary parameters for equation of state models.
- Binary parameters for Wilson, NRTL, and UNIQUAC models.
- Henry's law constants.
- Binary and pair parameters for electrolyte NRTL models.

For a specific parameter in a particular run, you may change the list and order on the Properties Parameters Binary Interaction and the Properties Parameters Electrolyte Pair folders.

Choosing Which Databanks are Searched

To move a databank to the Searched list:

1. Click the databank you wish to move.
2. Click the right arrow to move the databank to the Searched list.

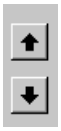
To move a databank from the Searched list:

1. Click the databank you wish to move.
2. Click the left arrow to move the databank to the Not Searched list.

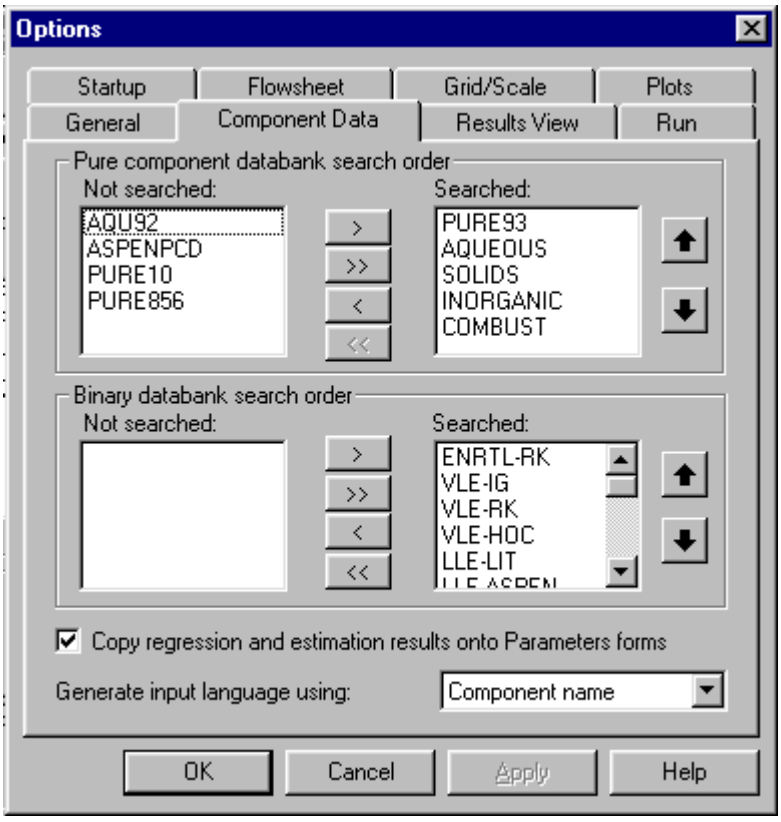
To move all of the databanks at once from one list to the other:

➤ Click the appropriate double arrow.

Reorder the databanks using the up and down arrows.



Example of Reordering Databanks



For pure component data, the PURE93 databank is searched first, the AQUEOUS databank is searched second and then, the SOLIDS, INORGANIC and COMBUST databanks are searched, in that order.

The AQU92, ASPENPCD, PURE10, and PURE856 databanks are not searched at all.

For binary data, the ENRTL-RK databank is searched followed by the VLE-IG, VLE-RK, VLE-HOC, LLE-LIT and LLE-ASPEN databanks.

Copying Regression and Estimation Results

You can retrieve regression or estimation parameter results and display them on the Parameters forms. To do this:

➤ On the Components Data tab, check the Copy regression and estimation results onto Parameters forms box.

The parameters will be used in all subsequent runs.

When this check box is clear, the parameters are available on the appropriate Physical Properties Parameters form, using the drop down list, but are not displayed on the forms. The parameters will not be used in subsequent runs.

Changing Defaults for Generating Input Language

You can use the Components Data tab to select whether you generate input language using Component name or Component alias.

Use the Formula column (up to 12 characters) or the Component Name column (up to 32 characters) on the Components Specifications Selection sheet to generate the COMPONENTS paragraph in the Aspen Plus input file.

Using the Results View Tab

Global data such as stream temperature and pressure can be viewed by selecting Global Data from the View menu. The data displayed can be customized using the Tools Options Results View tab.

For more information on using global data see Chapter 14.

The following parameters are available on the Results View tab:

Use this box	To	Saved with simulation
Output Units of Measurement	Select the units of measure for the global data output.	No
Heat/Work Variables	Specify if Heat or Work is shown (if available for streams) when global data is viewed. Use the Format box to specify the variable format.	Yes
Temperature	Specify if Temperature is shown (if available for streams) when global data is viewed. Use the Format box to specify the variable format.	Yes
Pressure	Specify if Pressure is shown (if available for streams) when global data is viewed. Use the Format box to specify the variable format.	Yes
Total Flow Rate	Specify if Total flow rate is shown (if available for streams) when global data is viewed. Use the Format box to specify the variable format.	Yes
Duty/Power	Specify if Duty or Power is shown (if available for heat and work streams) when global data is viewed. Use the Format box to specify the variable format.	Yes

† *These are shown if available for streams when global data is viewed.*

Format for Numbers

You can control the format of global data on the process flowsheet window. There are three conversion formats:

- %-xx.yye
- %-xx.yyf
- %-xx.yyg

This table explains the variables:

Variable	Explanation
%	Percent character. Lead character for format specification.
-	Optional minus sign, which left-justifies the number. Without the minus sign, the number is right-justified.
Xx	A digit string specifying a minimum field length for the converted number. The number takes at least this much space to print, and more if necessary.
Yy	A digit string specifying the precision, (that is, the number of digits) to be printed to the right of the decimal point.
E	Number is converted to the form [-]a.bbbbbbbe[+]cc. Length of b is specified by yy (Default is 6). Use upper case E in the format specification for upper case E in the printed numbers.
f	Number is converted to the form [-]aaa.bbbbbb. Length of b is specified by yy (Default is 6).
G	The shorter of %e or %f is used. Use upper case G in the format specification for upper case G in the printed numbers.

The recommended format is %0.f which prints whole numbers.

Other common formats used in stream tables are:

Format	Explanation
%10.0f	Whole numbers, with no decimal digits or exponents.
%10.nf	Numbers without exponents and with n digits to the right of the decimal point, if space permits. Decimal points line up, unless decimal digits have been eliminated in some numbers.

Using the Flowsheet Tab

Use the Tools Options Flowsheet tab to set various naming, display, and placement options on the Process Flowsheet.

The following parameters are available on this tab:

Use this box	To	Saved with simulation
Automatically Assign Block Name with Prefix	Have blocks automatically assigned a name beginning with the specified character string. For example, if B is entered, the blocks will be named B1, B2, B3, etc. When this option is off, Aspen Plus will prompt you to enter an ID each time a block is created.	Yes
Display Block Name	Have future block names displayed with the icon on the Process Flowsheet.	Yes
Automatically Assign Stream Name with Prefix	Have streams automatically assigned a name beginning with the specified character string. When this option is off, then Aspen Plus will prompt you to enter an ID each time a stream is created.	Yes
Display Stream Name	Have future stream names displayed on the streams in the Process Flowsheet.	Yes
Automatically Place Blocks When Importing	Automatically place blocks when importing a flowsheet Use this option to specify whether or not Aspen Plus automatically places any new blocks when you import an Aspen Plus backup file that does not contain graphics layout information. When this option is off, the Unplaced Blocks menu appears showing blocks that are not in the process flowsheet . You can later place these blocks automatically or manually. Blocks and streams already in the drawing and whose connectivity has not changed are not affected by this option. For more information on placing and unplacing blocks, see Chapter 4. For more information on importing a flowsheet, see Chapter 15.	Yes
Lock Block Spacing Factor at	Lock the block spacing factor at a specified value. A spacing factor of 2.5 is generally appropriate for flowsheets drawn with the block icons. For flowsheets drawn with pictorial icons, a factor of 1.5 is often better.	No

Continued

Use this box	To	Saved with simulation
Label Size Scale Factor	Control the size of block and stream IDs for printing. When Global Data is on, this factor also controls the size of the displayed global data values and legend box. This is a relative factor. Use a larger value for larger IDs and global data values. A factor between 2-3 is generally appropriate when printing relatively large flowsheets.	Yes

Using the Grid/Scale Tab

Use the Tools Options Grid/Scale tab to set and display the grid and scale on the process flowsheet window.

The following parameters are available on the Grid/Scale tab:

Use this box	To	Saved with simulation
Show Scale	Display a scale at the top and left of the process flowsheet window	Yes
Show Grid	Display the grid in the process flowsheet window. The grid lines can help you position objects, especially graphics and text objects. **Note** For the grid to be displayed, you must be zoomed in enough for the grid points to be distinguishable.	Yes
Snap to Grid	Align objects in the process flowsheet window to the grid when they are placed, moved, or resized	No
Grid Size	Specify the interval between grid points. When Snap to grid is on, inserted graphic objects are snapped to the grid lines. If you are zoomed in, you may want to decrease the grid resolution factor to position objects precisely. The grid sizes to choose from are 0.2, 0.1, 0.05, 0.025, 0.0125	Yes
Zoom Out Scale Factor	Set the degree for zooming in or out on the process flowsheet Values range from 1.0 to 10.0. A value of 10.0 will zoom out in greater increments than a value of 1.0.	No
Scroll Step Size	Set the percentage for scroll bar stepping[†] Scroll step affects only the scroll bars for the process flowsheet.	No

[†] *A scroll bar step is the amount that the screen scrolls with one mouse click a scroll bar arrow.*

Using the Plots Tab

Use the Tools Options Plots tab to specify the default fonts, grid style, line style, and marker size used when creating plots. This tab is also used to select if a legend and time stamp are displayed by default.

The following parameters are available on the Tools Options Plots tab:

Use this box	To	Saved with simulation
Default Fonts	Change the default font for the Title, Axis label, Axis scale, and Annotation	No
Grid Style	Define the type of grid for the plot. Mesh, Horizontal, Vertical, or No grid can be selected.	No
Line Style	Select the line style for the data curves. Lines & markers, Lines, or Markers can be selected.	No
Marker Size	Select the size for the markers. Values from 1-20 can be selected.	No
Show Legend	Show a legend	No
Show Time Stamp	Show a time stamp	No

Using the Run Tab

Use the Tools Options Run tab to select run options for interactive runs and specifications for a remote server.

The following parameters are available on the Tools Options Run tab:

Use this box	To	Saved with Simulation
Express Run	Use Express Run for maximum simulation speed when you run the Aspen Plus simulation engine on a PC, or interactively on other platforms. Express Run turns flowsheet animation off, and changes the Control Panel (terminal) message levels to 0. You can change the Control Panel message levels on the Setup Specifications Diagnostics sheet. If you change the Control Panel message levels on this sheet, and then turn on Express Run, Aspen Plus will not save the values you entered. When you turn Express Run off, all Control Panel message levels are set to 4.	

Continued

Use this box	To	Saved with simulation
Interactively Load Results	Load results only for objects you select in an interactive run When Interactively Load Results is off, Aspen Plus loads all simulation results into the Graphical User Interface at the end of the simulation. Interactively Load Results speeds up processing time by only loading the results you are interested in. It is useful if you run a simulation several times, but are only interested in the results on a few particular forms. When Interactively Load Results is on, you can still load all results using Check Results from the Run menu. Interactively Load Results only works with the Flowsheet Run type.	Yes
Animate Flowsheet During Calculations	Highlight blocks as they are executed during an interactive run Turning animation off can sometimes result in a slight increase in simulation speed.	Yes
Edit Keyword Input Before Starting Calculations	Edit the input language file before beginning an interactive run Aspen Plus displays the generated input language file in your editor before starting interactive calculations. This gives you a chance to make small modifications or additions to the file, or to diagnose problems. These modifications will not be reflected on the input forms. This feature is intended for advanced users who are familiar with keyword input language.	No
Server Type	Specify the Server type for remote server.	No
Server Name	Specify the name of the remote server.	No
Username	Specify the Username for the account on the remote server.	No
Working Directory	Specify the working directory on the remote server.	No

Using the Startup Tab

Use the Tools Options Startup tab to specify startup options for a new flowsheet.

The following parameters are available on the Tools Options Startup tab:

Use this box	To
Run Type	Select the default startup Run Type.
Application Template	Select the default application template
Working Directory	Select the default working directory for Aspen Plus simulation runs. All new files will be created in the specified working directory. This does not affect any existing files that you open - all the run files, including temporary ones, will be created in the directory where the file is.
Enable forms for layered products	Enable the forms for Aspen Plus layered products The forms for BatchFrac†, RateFrac, Aspen Dynamics, and POLYMERS PLUS can be enabled. This option is not available if the layered product is not installed.
Text Editor	Select the default text editor Specify the text editor to use for editing ASCII files that are obtained from the View Input Summary, History and Report commands from the View menu.
Print Text File Command	Select the command used to print

† *Rigorous 2 or 3 phase batch distillation process model. This model is not available in Aspen Plus Version 10, but will be available in Aspen Plus 10.1*

Using the Window Menu

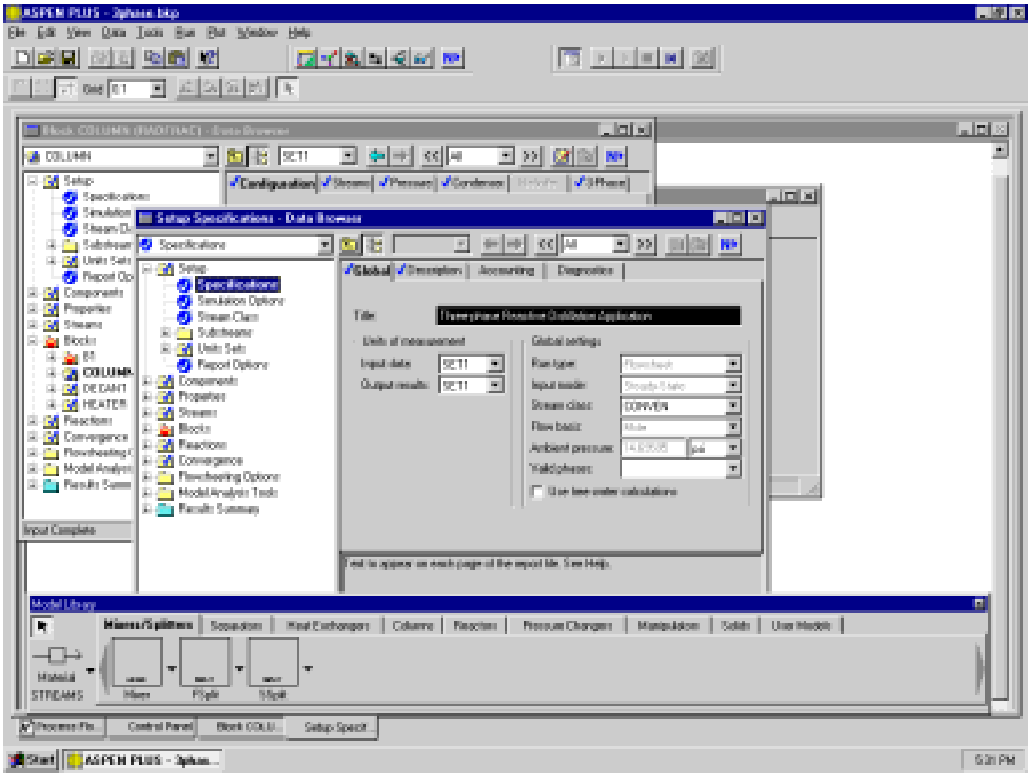
The following parameters are available on the Window menu:

Use this option	To
Cascade	Create a cascade of all of the open windows
Tile	Tile all of the open windows
Arrange Icons	Arrange the icons of any minimized windows
Normal	Display the Process Flowsheet in a normal window. The Process Flowsheet window can be moved, brought to the top and minimized.
Flowsheet as Wallpaper	Always keep the flowsheet fully open at the back of the program window Flowsheet as Wallpaper can only be used if Workbook Mode is off.
Workbook mode	Select if the Windows are displayed using Workbook mode Workbook mode can only be used if Flowsheet as Wallpaper is off.

Using Workbook Mode

Use Workbook mode to help organize all of your open windows.

In Workbook mode, each window has a tab that appears at the bottom of the screen. This makes it easy to see which windows are open.

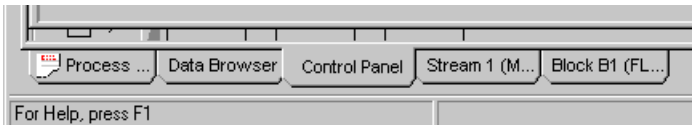


To use Workbook mode:

➤ From the Window menu, click Workbook Mode.

To make the desired window current:

➤ Click the appropriate tab at the bottom of your screen.



Tip You can also select any visible part of a window behind the current window by clicking it.

Customizing Application Template Files

An Application Template file contains simulation defaults commonly used by specific industries or companies. You can select an Application Template when you create a new run. You can use and modify a built-in file, or you can create your own Application Template files. For detailed information on the Application templates, see Chapter 2.

Use the built-in Application Templates as a guide when creating your own customized Application Template files.

There is no limit to the amount of information that can be included in a template: setup information, components, unit sets, property specifications, and even unit operation models can all be saved in a template if desired. Too much information may be inconvenient; however, objects or specifications in a template can be deleted if they are not needed in a simulation.

If you want to customize the stream summary format, you will need to create or modify a TFF file. For more information on how to create a TFF file, see Chapter 36.

Note Application Template files are not intended for problem specifications, such as when you want to save defaults or partial specifications for a particular process or unit. In such cases, create a backup file or an insert instead of an Application Template file.

Saving a Template File

To save an Aspen Plus template file:

1. From the File menu, select Save As.
2. Select Aspen Plus Templates (*.apt) from the Save as Type list.
3. Select the directory and enter a filename. The file can be in any directory.
4. Click Save.

Tip If you save your customized templates in a folder inside the Templates folder, they will appear as a separate tab on the New dialog box.

Tip The format for a Aspen Plus template file is the same as for a backup file; therefore, it is possible to create a template from a backup file by simple changing the extension from .bkp to .apt.

Importing a Template File

To import an Aspen Plus template file:

1. From the File menu, select Import.
2. Select Aspen Plus Template (*.apt) from the Files of Type list.
3. Select the directory and enter a filename. The file can be in any directory.
4. Click Open.
5. If the Resolve ID Conflict dialog box appears, there are objects that have the same ID as objects in the current run. For information on the Resolve ID Conflict dialog box, see Chapter 38.

Index

A

B

C

D

E

F

G

H

I

L

M

N

O

P

R

S

T

U

V

W