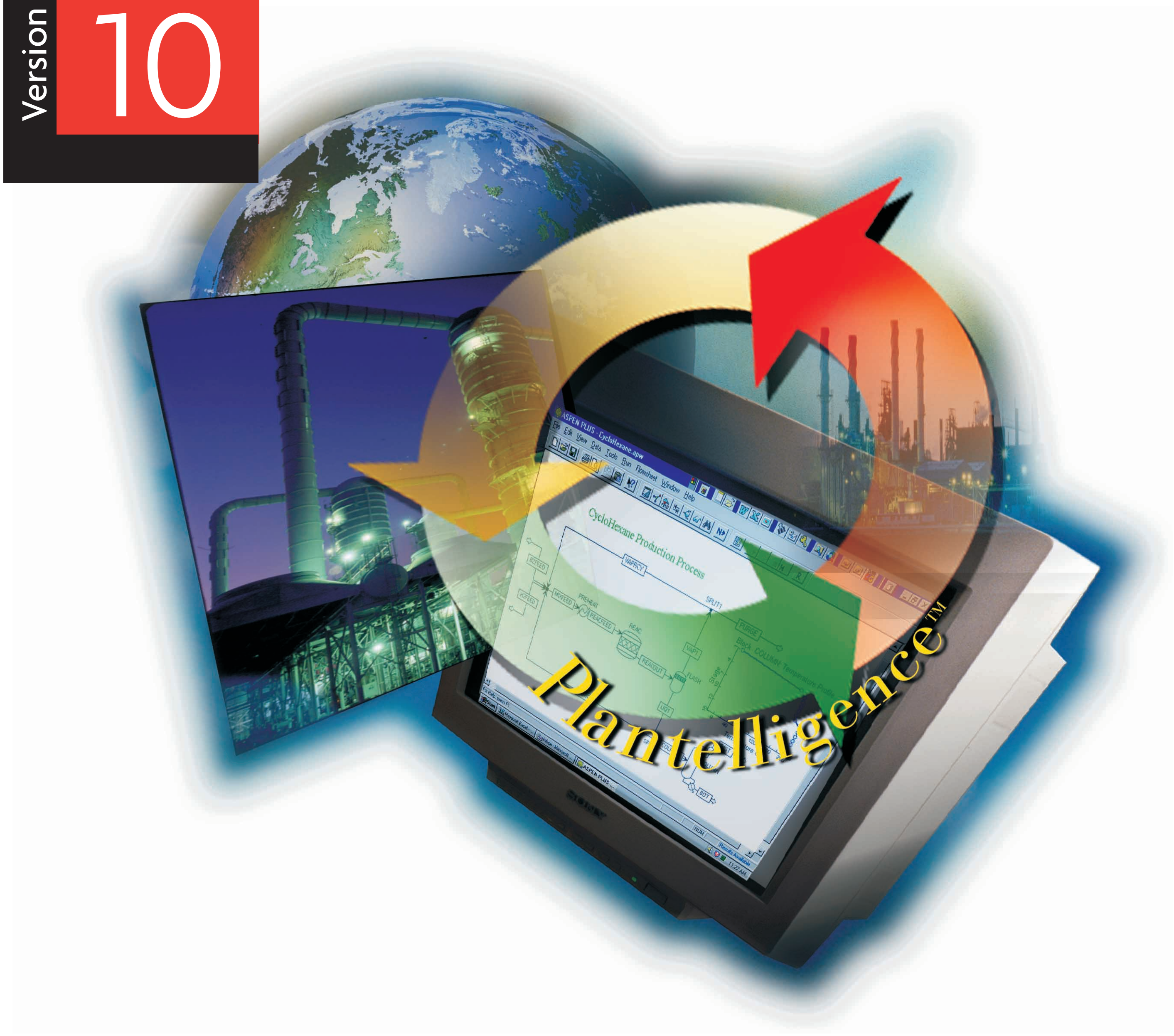
Aspen Plus®

STEADY STATE SIMULATION

Version 10



User Guide

AspenTech®

VOLUME 2

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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
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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
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(Brussels office)	+32-2/724-0100	+32-2/705-4034	
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17 Convergence

This chapter includes the following topics about convergence:

- Flowsheet recycles and design specifications
- Convergence Options
- Specifying tear streams
- User-defined convergence blocks
- Convergence Methods
- User-defined convergence order
- Specifying the calculation sequence
- Initial guesses
- Flowsheet sequencing
- Checking results
- Control panel messages
- Strategies for flowsheet convergence

Flowsheet Recycles and Design Specifications

Aspen Plus performs flowsheet calculations using the sequential modular method. Each unit operation block is executed in sequence. The calculated output streams of each block are used as feed to the next block.

Flowsheets with recycle loops, design specifications, or optimization problems must be solved iteratively. Execution requires that:

- Tear streams are chosen. A tear stream is a recycle stream with component flows, total mole flow, pressure, and enthalpy all determined by iteration. It can be any stream in a loop.

- Convergence blocks are defined to converge the tear streams, design specifications, or optimization problems. Convergence blocks determine how guesses for a tear stream or design specification manipulated variable are updated from iteration to iteration.
- A sequence is determined, which includes all of the unit operation and convergence blocks.

If you do not specify the tear streams, convergence blocks, or sequence, Aspen Plus determines them automatically. Every design specification and tear stream has an associated convergence block. The Aspen Plus generated convergence block names begin with the character “$.” User-defined convergence blocks should not begin with the character “$.”

Aspen Plus automatically determines any additional specifications needed to execute the flowsheet. By default, Aspen Plus also checks the user-specified sequences to ensure that all loops are torn.

Convergence specifications you can make are:

If you want to specify	Use this Convergence form	For more details see this section in this chapter
Convergence parameters and/or methods for convergence blocks	Conv Options	Convergence Options
Some or all of the tear streams needed for system-generated convergence blocks	Tear	Specifying Tear Streams
Some or all of the convergence blocks needed	Convergence	Specifying User-Defined Convergence Blocks
Convergence order for some or all of the user-defined convergence blocks	Conv Order	Specifying Convergence Order
Sequence for all or part of a flowsheet	Sequence	Specifying the Calculation Sequence

Convergence Options

Use the Convergence ConvOptions sheets to specify the following for convergence blocks:

- Tear Convergence tolerance
- Convergence methods for tear streams, design specifications, and optimization problems used in convergence blocks generated by Aspen Plus
- Parameters that affect sequencing
- Convergence parameters for each method. The specified parameters are used as defaults for convergence blocks you define and convergence blocks generated by Aspen Plus.

Specifying Tear Convergence Parameters

A tear stream is converged when the following is true for all tear convergence variables:

$$-tol \le \frac{X_{calculated} - X_{assumed}}{X_{assumed}} \le tol$$

For streams, the default convergence variables are total mole flow,all component mole flows, pressure, and enthalpy. When the Trace Option is Cutoff (specified on the Convergence ConvOptions Defaults TearConvergence sheet), Aspen Plus bypasses this convergence test for components that have a mole fraction less than the Trace threshold. The default Trace threshold is Tolerance/100. The alternative trace option, Trace-option = Gradual, adds a 100*Trace threshold term to the denominator. This setting gradually relaxes the convergence test for trace components.

To specify tear convergence parameters for convergence blocks:

1. From the Data menu, point to Convergence, then Conv Options.
2. Click the Tear Convergence sheet.
3. Specify tolerance and other convergence parameters, such as Trace Threshold and Trace Option.

The following parameters are available on the Tear Convergence sheet:

Field	Default	To
Tolerance	0.001	Specify Tear convergence tolerance A tear stream is converged when the following is true for all stream variables: $-tol \le \frac{X_{calculated} - X_{assumed}}{X_{assumed}} \le tol$
Trace Threshold	Tolerance/100	Specify the trace component threshold Aspen Plus bypasses this convergence test for components that have a mole fraction less than the Trace threshold.
Trace Option	Cutoff	Select the Convergence test option for trace components. Trace option = Gradual adds 100*TraceThreshold term to the denominator. This setting gradually relaxes the convergence test for trace components.
Component Group	All components	Identify the Component group ID for components to be converged in tear streams Component groups are defined on the Components Comp-Group form (see Chapter 6). Use a component group when you know that some components have zero or constant flow rates. A Component Group may cause convergence problems if the unconverged components have significant flow. Component group specifications are intended primarily for use with the matrix convergence methods (Broyden, Newton, and SQP) to reduce the matrix size and the number of numerical derivative perturbations.

Continued

Field	Default	To
State	Pressure & Enthalpy	Select the State variables to be converged. You can select a State option other than the default (Pressure and enthalpy) when pressure is known to be constant or enthalpy is not calculated (mass-balance-only simulations). State specifications are intended primarily for use with the matrix convergence methods (Broyden, Newton, and SQP) to reduce the matrix size and the number of numerical derivative perturbations.
Restore Tears on Error	checked	Restore tear to last guessed value when there is a convergence error.
Flash Tear Streams	checked	Flash tear streams after being updated by the convergence block. Check Flash Tear Streams if you access the temperature, density or entropy of the tear stream through in-line Fortran or if you need to see or use intermediate or partial convergence results. Do not check Flash Tear Streams if you want to save calculation time or if you do not need intermediate convergence results. Flashing tear streams is independent of the convergence method, with one exception. If Chemistry is associated with the tear stream, then the default is not to flash for tear streams, irrespective of your selection.
Diagnostics	Display Maximum Error / Tolerance	Specify whether tables of all variables or only the variable with the maximum error should be generated.

Specifying Default Methods

You can specify the numerical methods to be used by the system-generated convergence blocks. See Convergence Methods, this chapter, for information on the numerical methods.

To specify the numerical methods to be used by the system-generated convergence blocks:

1. From the Data menu, point to Convergence, the Conv Options.
2. Select the Default Methods sheet.
3. You can specify the numerical methods to be used by the convergence blocks.

The following parameters are available on the Default Methods sheet:

Field	Default	To specify the convergence method for system-generated
Tears	Wegstein	Tear convergence blocks The other methods available are Direct, Broyden, and Newton.
Single Design Spec	Secant	Single design-spec convergence blocks The other methods available are Broyden and Newton.
Multiple Design Specs	Broyden	Multiple design-spec convergence blocks The other method available is Newton.
Tears & Design Specs	Broyden	Combined tears and design-specs convergence blocks The other method available is Newton.
Optimization	SQP	Optimization convergence blocks

Specifying Sequencing Parameters

You can specify parameters to control tear stream selection and automatic sequencing.

To specify the tearing and sequencing parameters:

1. From the Data menu, point to Convergence, then Conv Options.
2. Select the Sequencing sheet.
3. You can specify the tearing and sequencing parameters.

The following parameters are available on the Sequencing sheet:

Field	Default	To specify
Design Spec Nesting	Inside	Whether design specifications should be nested inside tear stream loops, outside tear stream loops, or converged simultaneously with tear streams Design Spec Nesting does not apply to convergence blocks specified in the Convergence Order form. When the tear of an outer loop is recalculated in an inner loop, the actual sequence generated may not strictly follow the loop-order preference specified in the Design Spec Nesting and User Nesting fields.
User Nesting	Outside	User Nesting lets you specify a preference for whether convergence blocks specified on the Conv Order form should be nested inside or outside other convergence blocks (user-defined or system-generated) The User Nesting field has precedence over the Design Spec Nesting field. When the tear of an outer loop is recalculated in an inner loop, the actual sequence generated may not strictly follow the loop-order preference specified in the Design Spec Nesting and User Nesting fields.

Continued

Field	Default	To specify
Variable Weight	1	Tear variable weighting factor for tearing algorithm If Variable Weight is a large number, the tearing algorithm minimizes the number of torn variables.
Loop Weight	1	Loop weighting factor for tearing algorithm If Loop Weight is a large number, the tearing algorithm minimizes the number of loops torn.
Tear Fortran Write Variables	not checked	Whether Fortran block variables can be torn when Fortran blocks appear in feedback loops See Chapter 19, Fortran, in the section,Converging Loops Introduced by Fortran Variables for more information and an example
Check Sequence	checked	Whether Aspen Plus checks a user-specified sequence to ensure that all loops are torn

Specifying Convergence Method Parameters

You can specify additional parameters for each numerical method. Select the appropriate tab for the convergence method. See Convergence Methods, this chapter, for information on the numerical methods.

To specify the additional parameters:

1. From the Data menu, point to Convergence, then Conv Options.
2. In the left pane of the Data Browser window, select the Methods form.
3. Select the appropriate sheet for the convergence method.
4. Specify the parameters for that method.

Specifying Tear Streams

Use the Tear Specifications sheet to identify tear streams to be converged by system-generated convergence blocks. If you specify an incomplete tear set for your flowsheet, Aspen Plus automatically chooses the remaining set of streams. If you specify a redundant tear set (too many tear streams), Aspen Plus may ignore some tears or find an inefficient sequence.

To specify a tear stream:

1. From the Data menu, point to Convergence, then Tear.

2. In the Stream field, use List and select a stream ID.

   The stream must be in a recycle loop in the simulation flowsheet.

   Note When a Fortran block is in a recycle loop, you can tear variables designated as Write Variables on the Fortran Sequence sheet.

3. Specify any of the remaining optional fields, as you choose.

   The following parameters are available on the Tear Specifications sheet:

Field	Default	To
Tolerance	0.001	Specify Tear convergence tolerance A tear stream is converged when the following is true for all stream variables: $-tol \le \frac{X_{calculated} - X_{assumed}}{X_{assumed}} \le tol$
Trace	Tolerance/100	Specify the trace component threshold Aspen Plus bypasses this convergence test for components that have a mole fraction less than the Trace threshold.
Component Group	All components	Identify the Component group ID for components to be converged in tear streams Component groups are defined on the Components Comp-Group form (see Chapter 6). Use a component group when you know that some components have zero or constant flow rates. A Component Group may cause convergence problems if the unconverged components have significant flow. Component group specifications are intended primarily for use with the matrix convergence methods (Broyden, Newton, and SQP) to reduce the matrix size and the number of numerical derivative perturbations.
State	Pressure & Enthalpy	Select the State variables to be converged You can select a State option other than the default (Pressure and enthalpy) when pressure is known to be constant or enthalpy is not calculated (mass-balance-only simulations). State specifications are intended primarily for use with the matrix convergence methods (Broyden, Newton, and SQP) to reduce the matrix size and the number of numerical derivative perturbations.

Initial Estimates for Tear Streams

You can use the Stream sheets to provide an initial estimate for the tear stream. An initial estimate generally aids recycle convergence, and is sometimes necessary, especially for recycle loops involving distillation blocks. For more information on specifying streams see Chapter 9.

Specifying User-Defined Convergence Blocks

Use the Convergence sheets to specify convergence method, tolerance, and convergence variables for user-defined convergence blocks. System-generated convergence blocks generated by Aspen Plus do not use these specifications.

To define a convergence block:

1. From the Data menu, point to Convergence, then Convergence.
2. In the Convergence Object Manager click New.
3. In the Create New ID dialog box, enter an ID or accept the default name.
4. In the Create New ID dialog box, select the type of convergence block you want to create.

Use this method	To converge
BROYDEN or NEWTON	Tear streams; two or more design specifications; or tear streams and design specifications simultaneously. Use when the recycle loops and/or design specifications are highly interrelated. Use Newton when Broyden is unable to converge.
COMPLEX	Optimization with inequality constraints
DIRECT	Tear streams by simple direct substitution. Convergence may be slow, but sure.
SECANT	Single design specifications. Recommended for design specification convergence blocks.
SQP	Sequential quadratic programming. Optimization with any combination of tear streams, equality constraints, and inequality constraints.
WEGSTEIN	Tear streams. You can apply Wegstein to any number of streams simultaneously. Recommended tear stream convergence method.

For more information on the numerical methods, see Convergence Methods, this chapter.

5. Click the Tear Streams, Design Specifications, Fortran Tears or Optimization tab to select the elements that you want the convergence block to solve.
6. To specify optional parameters, click the Parameters sheet.

Convergence Methods

This section describes the convergence methods available in Aspen Plus.

The parameters for each method can be found on the Convergence ConvOptions Methods form and on the form for the Convergence block.

WEGSTEIN Method

The classical bounded Wegstein method is usually the quickest and most reliable method for tear stream convergence. It is an extrapolation of Direct substitution iteration. Interactions between variables are ignored; therefore, it does not work well when variables are strongly coupled.

Wegstein method can only be used for Tear streams. It is the default method for Aspen Plus tear stream convergence. Apply it to any number of streams simultaneously. You can control the Wegstein bounds and the frequency of acceleration.

You can control the Wegstein method by specifying:

Field	Default	To specify the
Maximum Flowsheet Evaluations	30	Maximum number of flowsheet evaluations
Wait	1	Number of direct substitution iterations before the first acceleration iteration
Consecutive Direct Substitution Steps	0	Number of direct substitution iterations between acceleration iterations
Consecutive Acceleration Steps	1	Number of consecutive acceleration iterations
Lower Bound	-5	Minimum value for the Wegstein acceleration parameter (q)
Upper Bound	0	Maximum value for the Wegstein acceleration parameter (q)

Wegstein Acceleration Parameter

You can control the Wegstein method by specifying upper and lower limits for:

- Acceleration parameter q (Upper Bound and Lower Bound)
- Number of direct substitution iterations before the first acceleration (Wait)
- Number of direct substitution iterations between acceleration iterations (Consecutive Direct Substitution Steps)
- Number of consecutive acceleration iterations (Consecutive Acceleration Steps).

In the bounded Wegstein method, the acceleration parameter q is calculated for each tear stream variable as follows:

$$q = \frac{s}{s-1}$$

$$s = \frac{G(X_k) - G(X_k - 1)}{X_k - X_{k-1}}$$

Where:

X = Estimate of the tear stream variable

$G(X)$ = Resulting calculated value of the variable

k = Iteration number

The new estimate calculated by Wegstein is:

$$\begin{aligned} X_{k+1} &= qX_k + (1-q)G(X_k) \\ &= X_k + (1-q)(G(X_k) - X_k) \end{aligned}$$

The following shows the effect of q on convergence:

q	Convergence
q < 0	Acceleration
q = 0	Direct substitution
0 < q < 1	Damping

Because oscillation or divergence can occur if q is unbounded, limits are set on q. The default lower and upper bounds on q are -5 and 0, respectively. For most flowsheets, these limits work well and do not need to be changed.

Normally, you should use an Upper Bound of the Wegstein acceleration parameter of 0. If iterations move the variables slowly toward convergence, smaller values of the lower bound of the Wegstein acceleration parameter (perhaps -25 or -50) may give better results. If oscillation occurs with direct substitution, values of the lower and upper bounds between 0 and 1 may help.

DIRECT Method

For direct substitution, the new value of the tear stream variable is the value resulting from the previous flowsheet calculation pass:

$$X_{k+1} = G(X_k)$$

Where:

X = Estimate of tear stream variable

$G(X)$ = Resulting calculated value of the variable

k = Iteration number

With direct substitution, convergence is slow but sure. It is available for those rare cases where other methods may be unstable. Direct substitution can also make it easy to identify convergence problems, such as component build-up in the system. Direct substitution is equivalent to Wegstein with lower bound=upper bound=0.

Secant Method

Secant is the secant linear approximation method, with higher order enhancements. You can select a bracketing/interval halving option. Select this option whenever the function is discontinuous, non-monotonic, or flat over a region. Bracketing will eliminate the flat region and switch back to Secant method if possible.

You can use Secant for converging single design specifications. Secant is the default method for design specification convergence, and is recommended for user-generated convergence blocks.

You can control the Secant method by specifying:

Field	Default	To specify
Maximum Flowsheet Evaluations	30	Maximum number of flowsheet evaluations
Step Size	0.01	Initial step size, as a fraction of range, for the design specification manipulated variable
Maximum Step Size	1	Maximum step size, as a fraction of range, for the design specification manipulated variable

Continued

Field	Default	To specify
X Tolerance	1e-8	Alternative tolerance on the manipulated variable Iteration stops when the change in the scaled manipulated variable is less than X Tolerance.
X Final on Error	Last value	Which value of manipulated variable to use as the final value when the convergence block encounters an error Options are Last value, Initial value, Minimum value of function, Lower bound, and Upper bound.
Bracket	No	If the Secant algorithm should switch to a Bracketing algorithm. Bracketing attempts to find a variable range where the design specification function changes sign and performs interval halving when Secant is not making progress. When Bracket is specified as No, then Bracketing is not used. Since bracketing may add extra iterations, in some cases, particularly with a nested secant loop, you might want to specify Bracket as No. When Bracketing is specified as Yes, Bracketing is tried if the function is not changing. The Bracket = Yes option is useful for functions that are flat over a portion of the variable range. When Bracket is specified as Check Bounds, Bracketing is tried if the function is not changing or if the Secant algorithm has moved to a variable bound. The Bracket = Check Bounds option is useful for functions that are flat over a portion of the variable range. It can also be useful for non-monotonic functions. This option ensures that if the Secant algorithm becomes stuck at a variable bound, the other variable bound will also be tried.
Find Minimum Function Value if Bracketing Fails to Detect a Sign Change.	Not checked	Find the minimum function value if bracketing fails to detect a sign change.

BROYDEN Method

The Broyden method is a modification of Broyden's quasi-Newton method. The Broyden method is similar to the Newton method, but it uses approximate linearization. This approximation makes Broyden faster, but occasionally not as reliable, as the Newton method.

Use Broyden to converge tear streams, two or more design specifications, or tear streams and design specifications simultaneously. Broyden is useful for multiple tear streams and/or design specifications, tear variables that are highly interdependent, or recycle loops and design specifications so interrelated that nesting is impractical. When converging both tear streams and design specifications, you can specify that tear streams be converged or partially converged first. The simultaneous convergence of both tear streams and design specifications then follows.

You can control the Broyden method by specifying:

Field	Default	To specify
Maximum Flowsheet Evaluations	30	Maximum number of flowsheet evaluations
X Tolerance	0.001	Alternative tolerance on the manipulated variables The iteration stops when the change in the scaled manipulated variable is less than X Tolerance
Wait	2	Number of direct substitution iterations before the first acceleration iteration
Tear Tolerance (on Advanced Parameters dialog box)		Tear tolerance. Used if initializing tears by converging tears (to specified tolerance) before design specifications are included
Tear Tolerance Ratio (on Advanced Parameters dialog box)		Tear tolerance ratio. Used if initializing tears by converging tears (to a tolerance relative to the tear tolerance) before design specifications are included
Maximum Iterations (on Advanced Parameters dialog box)		Maximum number of flowsheet iterations to solve tears before design specifications are included
Lower Bound (on Advanced Parameters dialog box)	-5	Minimum value for the Wegstein acceleration parameter (q)
Upper Bound (on Advanced Parameters dialog box)	0	Maximum value for the Wegstein acceleration parameter (q)

NEWTON Method

NEWTON is an implementation of the modified Newton method for simultaneous nonlinear equations. Derivatives are calculated only when the rate of convergence is not satisfactory. The implementation allows bounds on the variables, and includes a line search for improved stability. NEWTON is useful when the recycle loops and/or design specifications are highly interrelated, but convergence is not achieved using the Broyden method. Numerical derivatives are calculated frequently. Use NEWTON for tear streams only when the number of components is small or when convergence cannot be achieved by the other methods. When converging both tear streams and design specifications, you can specify that tear streams be converged or partially converged first. The simultaneous convergence of both tear streams and design specifications then follows.

When you use the Newton or Broyden methods to converge design specifications, and one or more manipulated variables have reached their lower or upper limits, a solution is found that minimizes the sum of squares of design specification and tear stream errors, divided by their tolerances. Iterations stop when the root mean square of the changes in the scaled manipulated variables is less than X tolerance. Aspen Plus scales each manipulated variable, dividing it by the absolute value of the lower or upper limit, whichever is larger.

You can control the Newton method by specifying:

Field	Default	To specify
Maximum Newton Iterations	30	Maximum number of Newton iterations
Maximum Flowsheet Evaluations	9999	Maximum number of flowsheet evaluations
Wait	2	Number of direct substitution iterations before the first acceleration iteration
X Tolerance	0.0001	Alternative tolerance on the manipulated variables The iteration stops when the change in the scaled manipulated variable is less than X Tolerance
Reduction Factor	0.2	Reduction factor which determines the number of Newton iterations used before calculating a new Jacobian (derivative) matrix With this option, the Jacobian is reused as long as it continues to decrease the error each iteration by the Reduction Factor
Iterations to Reuse Jacobian		Number of iterations to reuse the Jacobian (derivative) matrix With this option, the Jacobian is reused a set number of times The default is to base the reuse of the Jacobian on the Reduction Factor
Tear Tolerance (on Advanced Parameters dialog box)		Tear tolerance. Used if initializing tears by converging tears (to specified tolerance) before design specifications are included

Continued

Field	Default	To specify
Tear Tolerance Ratio (on Advanced Parameters dialog box)		Tear tolerance ratio. Used if initializing tears by converging tears (to a tolerance relative to the tear tolerance) before design specifications are included
Maximum Iterations (on Advanced Parameters dialog box)		Maximum number of flowsheet iterations to solve tears before design specifications are included
Lower Bound (on Advanced Parameters dialog box)	-5	Minimum value for the Wegstein acceleration parameter (q)
Upper Bound (on Advanced Parameters dialog box)	0	Maximum value for the Wegstein acceleration parameter (q)

COMPLEX Method

You can use the Complex method to converge optimization problems with bounds on the manipulated variables and inequality constraints. COMPLEX is a direct search method; it does not require numerical derivatives. It may be useful for simple problems without recycle loops or equality constraints (design specifications).

SQP Method

You can use the state-of-the-art sequential quadratic programming (SQP) method for flowsheet optimization for simultaneous convergence of optimization problems with constraints (equality or inequality) and/or tear streams. The algorithm generally follows an infeasible path (constraints and tear streams are converged simultaneously with the optimization problem). But you can adjust it to follow a feasible path (converging the tear streams at each iteration of the optimization). SQP is used for system-generated optimization convergence blocks. SQP is recommended for user-generated convergence blocks.

SQP-Biegler is an SQP implementation developed by Professor L. Biegler of Carnegie-Mellon University and his students.

You can control the SQP method by specifying:

Field	Default	To specify
Maximum Optimization Iterations	30	Maximum number of SQP optimization iterations
Maximum Flowsheet Evaluations	9999	Maximum number of flowsheet evaluations Each perturbation step for numerical derivatives is counted as one evaluation.
Additional Iterations when Constraints are not Satisfied	2	Number of additional iterations when constraints are not satisfied after the convergence test is satisfied.
Iterations to Converge Tears for Each Optimization Iteration	3	Number of iterations to take toward converging tears at each iteration of the optimization
Iterations to Enforce Maximum Step Size	3	Number of iterations to enforce maximum step size on the manipulated variables
Tolerance	0.001	Optimization convergence tolerance
Wait	1	Number of direct substitution iterations before the first acceleration iteration
Lower Bound	-5	Minimum value for the Wegstein acceleration parameter (q)
Upper Bound	0	Maximum value for the Wegstein acceleration parameter (q)

SQP Wegstein Acceleration Parameters

When the SQP method is used to converge tears and optimization problems simultaneously, the algorithm is a hybrid of an infeasible path method (where the tears are not converged at each iteration but are converged at the optimum) and a feasible path method (where the tears are converged at each iteration of the optimization). You may control the degree to which the tears are converged by specifying the number of iterations to take toward converging the tears (Iterations To Converge Tears Each Optimization Iteration) and upper and lower limits for the Wegstein acceleration parameter for the Wegstein iterations (Upper Bound, Lower Bound).

Specifying Convergence Order

You can specify the calculation order of convergence blocks you define if you use more than one user-defined convergence block. Specify the convergence order on the ConvOrder Specification or Sequence Specifications sheet.

To define a convergence order:

1. From the Data menu, point to Convergence, then Conv Order.
2. Select a block from the Available Blocks list. Use the arrow to move the block that you want converged first to the top of the Convergence Order list.
3. Select any other blocks that you want in the order and move them to the Convergence Order list. You can use the up and down arrows to rearrange the order within the list. The first convergence block is converged first and nested most deeply.

Specifying the Calculation Sequence

You can define the calculation order for all or part of the flowsheet. You supply an ID for each sequence.

To define a sequence:

1. From the Data menu, point to Convergence, then Sequence.
2. In the Object Manager click the New button.
3. In the Create New ID dialog box, enter an ID or accept the default ID and click OK.
4. Specify the calculation sequence on the Specifications sheet. On each row of the sheet, you can enter one of the following:
    - The beginning of a loop
    - The end of a loop
    - A block ID
    - A sequence ID for part of a flowsheet

For the beginning and end of a loop, specify Begin or Return To in the Loop-Return field. Specify the block type in the Block Type field. The following blocks begin loops:

- Convergence
- Sensitivity
- Data Fit

Fortran blocks can introduce loops only for the special case of loop control Fortran blocks.

Specify the block type and block ID for the following block types:

- Unit operation
- Equipment
- Utility
- Transfer

- Fortran
- Balance
- Pres-Relief

For economic calculations, specify Economic for block type. There is no block ID for economic calculations.

Within a sequence you can insert a subset of the flowsheet that already has an ID and a defined sequence. For large flowsheets it is useful to build up the sequence specification in this manner. Specify Sequence in the Block Type field. Specify the sequence ID for the subset in the Block ID field.

Aspen Plus executes the sequences exactly as you enter them, with these exceptions:

If you	Aspen Plus
Check the Check Sequence field on the ConvOptions Defaults Sequencing sheet	Checks whether all loops in a sequence are torn. If a loop is not torn, Aspen Plus displays an error message
Specify Execute Before or Execute After in a Fortran block	Inserts the Fortran block into your sequence
Specify a Design-Spec	Automatically generates convergence blocks for design specifications and inserts them into your sequence

Using Initial Guesses

For many simulations with recycle streams, initial guesses for the tear streams will help convergence. This is especially true for recycle systems with closed loops or recirculating solvent loops. You can often provide a reasonable initial guess from your knowledge of the process or through a simple mass-balance calculation.

The sequence is displayed in the left pane of the Control Panel. If the left pane of the Control Panel is empty, select Step from the Run menu.

Enter initial compositions and flow rates for the tear streams on Streams Specification sheets, and run the simulation. Or select your own tear streams using the Tear sheet, and provide initial estimates for them.

Flowsheet Sequencing

The tearing and sequencing of a flowsheet is complex and can require user input. The following information on interacting with the Aspen Plus sequencing algorithm is intended for advanced users. It is recommended that other users accept the default sequencing.

Aspen Plus initially tears and sequences flowsheets in this sequence:

1. The information flow (incidence matrix) of unit operation blocks, Fortran blocks, design specifications, constraints, optimizations, and cost blocks is collected.
2. Sequences you specify are checked for possible missing tears and are used to generate a reduced incidence matrix. In the reduced incidence matrix, subsequences you specify are collapsed and treated as a single block.
3. The reduced incidence matrix is partitioned into independent subsystems that can be solved sequentially.
4. Tear streams or Fortran block tear variables are determined for each subsystem, taking user-specified Tear, Tear Variable, and Convergence specifications into consideration. The automatic sequencing algorithm in Aspen Plus selects tear streams by minimizing a weighted combination of the number of:
    - Tear variables
    - Times loops are torn
5. An initial sequence is determined as part of the tearing. For each subsystem, Convergence blocks are created for design specifications, tear streams, and tear variables that are not converged by user-specified convergence blocks. Specifying Design Spec Nesting as Inside on the Convergence ConvOptions Defaults Sequencing sheet generates one tear convergence block for all tear streams and tear variables, and generates an individual design specification convergence block for each design specification. See Specifying Sequencing Parameters, this chapter, for more information.

You can affect the automatic sequencing algorithm by:

- Adjusting the Variable Weight and Loop Weight parameters on the Convergence ConvOptions Defaults Sequencing sheet.
- Specifying initial estimates for possible tear streams on the Streams forms. The specifications for non-feed streams are used as initial guesses if possible. Streams with data are weighted in the sequencing algorithm, so they are more likely to be selected as tear streams.
- Specifying tear streams directly, using the Tear Specification sheet. You should be careful not to specify more tear streams than required for convergence. You can underspecify the number of tear streams, and Aspen Plus will determine the additional tear streams needed.

Obtaining Final Convergence Sequence

To obtain the final convergence sequence:

1. All convergence blocks are ordered as they appear on the ConvOrder Specification form and the current setting of User nesting on the ConvOptions Defaults Sequencing sheet. Blocks not mentioned on the ConvOrder Specification form are ordered according to the setting of Design Spec Nesting on the ConvOptions Defaults Sequencing sheet and the span of convergence blocks in the initial sequence.
2. Aspen Plus obtains the final convergence sequence by repeatedly removing tears and/or design specifications from the outermost convergence block and partitioning the reduced flowsheet.
3. For Design specification nesting as Inside or Inside simultaneous on the Convergence ConvOptions Defaults Sequencing sheet, you can define user-specified convergence blocks for design specifications, and they will be inserted automatically into the sequence.

Adding Special Options to the Sequence

At the end of the final convergence sequence, special options are added:

1. Blocks with Execute options are inserted into the sequence.
2. Sensitivity, Balance, and Data Fit blocks not already in the sequence are inserted.

Because a design specification loop usually has a small span, the sequencing algorithm does not nest them (for example, a tear loop outside and many independent design specification loops inside). Since the algorithm does not take numerical values into account, it sometimes places design specification loops inside tear loops when they would perform better outside. Specifying Design Spec Nesting as Outside on the Convergence ConvOptions Defaults Sequencing sheet would alter the sequence but this often leads to deeply nested iteration loops for large flowsheets.

Viewing the Sequence

To view the sequence along with the tear streams and the convergence blocks determined by Aspen Plus:

➤ From the View menu, click Control Panel.

The sequence is displayed in the left pane of the Control Panel. If the left pane of the Control Panel is empty, select Step from the Run menu.

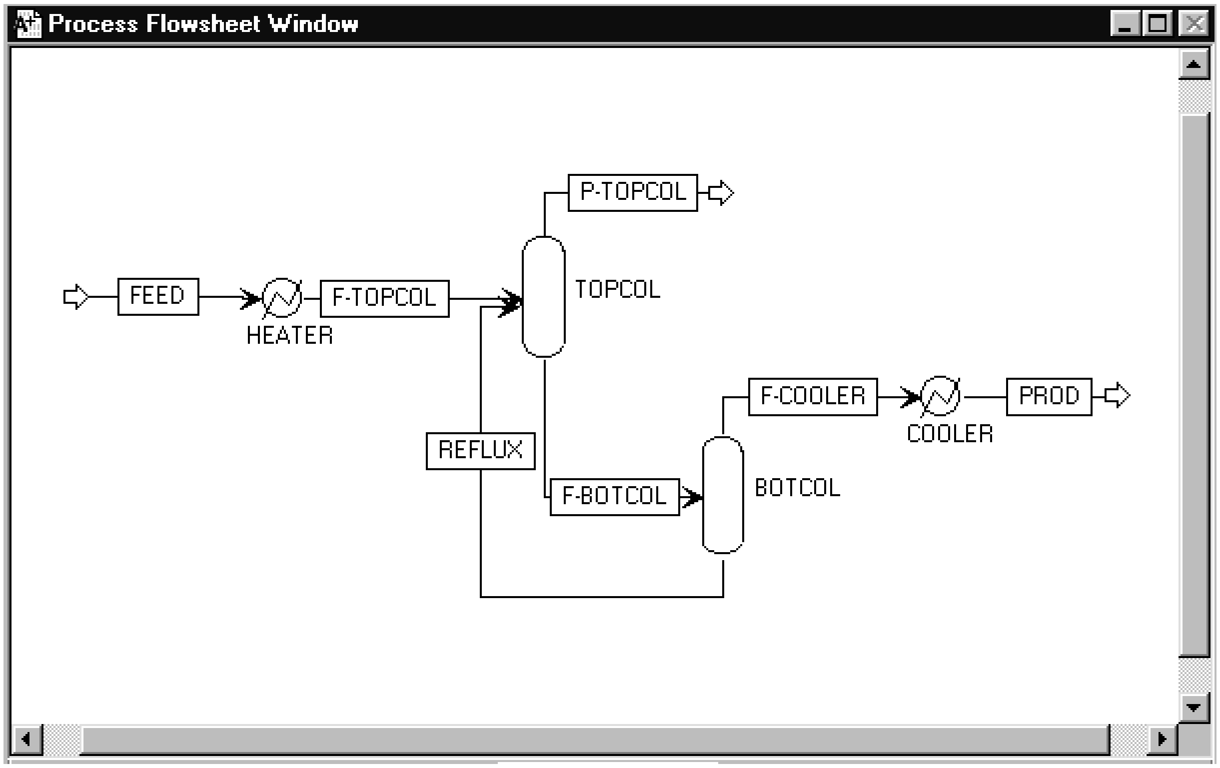
Sequencing Example

This example describes steps to converge a simple flowsheet that does not converge properly when automatic sequencing is used. It illustrates:

- Supplying initial estimates for recycle streams
- Altering the calculation sequence with Design spec nesting
- Altering the calculation sequence with Conv Order
- Adjusting tolerances to account for nested loops

The flowsheet consists of:

Blocks	Type
TOPCOL, BOTCOL	Interconnected columns
HEATER	Pre-heater
COOLER	Product cooler



The mass flow of stream REFLUX, the inter-reflux stream from BOTCOL to TOPCOL, is manipulated to meet a purity specification of component THF in stream PROD. PROD is a product stream from BOTCOL/COOLER, in design specification THF. PSPEC is the convergence block defined to converge THF.

When distillation columns appear in a recycle loop, it is often necessary to give initial estimates for the tear stream. Aspen Plus makes this easy. Simply supply data for a column feed or other stream in the loop on Streams forms, just as you would for a feed stream, and Aspen Plus will preferentially select the stream as a tear stream (your stream may not be selected if another stream is a better choice by the tearing criteria).

From initial estimates for the tear stream, the Aspen Plus sequencing algorithm determines the following computation sequence:

```
HEATER
$OLVER01 TOPCOL
|    PSPEC BOTCOL COOLER
|    (RETURN PSPEC)
(RETURN $OLVER01)
```

$OLVER01 is defined to converge stream REFLUX, the inter-connecting stream, with initial data provided. However, with this sequence the PSPEC and $OLVER01 convergence blocks fail to converge, because the design specification is nested inside the column recycle loop. The design specification THF does not converge, because the purity specification is determined primarily by the inter-reflux between the two columns (not the top product rate of the BOTCOL alone).

The inter-reflux between the columns should be converged before evaluation of the design specification. The design specification should be nested outside the column recycle loop. You can alter the nesting order of the convergence loops by either:

- Specifying Design Spec Nesting as Outside on the Convergence ConvOptions Defaults Sequencing sheet, or
- Specifying PSPEC on the Convergence ConvOrder Specifications sheet.

Either specification would cause the sequencing algorithm to determine the following computation sequence, which converges:

```
HEATER
PSPEC
|    $OLVER01 TOPCOL BOTCOL
|    (RETURN $OLVER01
|    COOLER
(RETURN PSPEC)
```

Both methods of specifying the nesting order are equivalent for this simple problem. But using the ConvOptions Defaults Sequencing form allows you to change the computation sequence selectively when dealing with large flowsheets.

In this flowsheet there is no need for special tolerance adjustments to account for the nesting of iteration loops. For some flowsheets it is necessary to adjust tolerances so the inner loops are calculated more accurately than outer loops; otherwise the outer loops would be overwhelmed with errors from inner loops. For the sequence above, use the following levels of calculation accuracy:

For these blocks	Use this level of accuracy
HEATER, PSPEC	Final
$OLVER01, COOLER	Intermediate (higher)
TOPCOL, BOTCOL	Highest

If the Error/Tolerance for PSPEC seems to go down to 10 quickly and stay there, you should tighten tolerances for all the blocks inside the PSPEC loop or loosen the tolerance for PSPEC. If you observe a similar problem in $OLVER01, you could tighten the tolerances of TOPCOL and BOTCOL.

It is particularly important to ensure that any nested design specifications have sufficiently tight tolerances, since these tolerances are specified by the user. If problems occur, or if the design specification is nested deeply, a tighter tolerance may be necessary.

Checking Convergence Results

After your simulation has completed or while it is paused, you can view convergence block results to check the status or diagnose convergence problems.

1. If your simulation is paused, from the Run menu, click Load Results.
2. On the Data menu, point to Convergence, then Convergence.
3. In the Convergence Object Manager, select the convergence block and click Edit. For system-generated convergence blocks, (names beginning with $OLVER), the results sheets are displayed. For user-defined convergence blocks, select Results on the left pane of the Data Browser window to display the results sheets.
4. Choose the appropriate sheet:

This sheet	Contains the information
Summary	Final convergence status, variable value, and Err/Tol for each variable converged by the block
Tear History	Table of maximum Err/Tol versus iteration number. Variable with maximum error at each iteration. Plots of Err/Tol versus iteration number can be generated.
Spec History	Table of manipulated variable values and design specification error versus iteration number. You can generate plots of design specification error versus iteration number, or design specification error versus manipulated variable value.

Use the Tear History and Spec History sheets and the Diagnosing Tear Stream Convergence and Diagnosing Design-Spec Convergence tables, to help you diagnose and correct tear stream and design specification convergence problems. It is helpful to generate a plot of Err/Tol versus iteration number.

Increasing diagnostics can also help with diagnosing problems. See Convergence Diagnostics, this chapter, for more information.

Control Panel Messages

The Control Panel displays convergence diagnostics for each convergence block. Each time the convergence block is executed in a recycle convergence loop, messages appear with the following format:

```
> Loop CV          Method: WEGSTEIN Iteration 9
Converging tear streams: 3
4 vars not converged, Max Err/Tol    0.18603E+02
```

Each time a convergence block for a design specification is executed in a convergence loop, messages appear with the following format:

```
>> Loop CV         Method:  SECANT Iteration 2
Converging specs:  H2RATE
1 vars not converged, Max Err/Tol    0.36525E+03
```

Where:

CV = Convergence block ID

Max Err/Tol = Maximum error/tolerance for the unconverged variables

\> = Symbol indicating nesting level of the convergence loop
- \> Outside loop
- \>> Loop nested one deep
- \>>> Loop nested two deep
- and so on

Convergence is achieved when the value of Max Err/Tol becomes less than 1.0.

Convergence Diagnostics

You can modify the diagnostic level for convergence globally on the Setup Specifications Diagnostics sheet. For more details about how to change the diagnostics level, see Chapter 5.

Use the Convergence sliders to modify the diagnostic level for convergence block information in either the control panel and in the history file. You can also specify the diagnostic level for a single convergence block using the Diagnostics button on the Input Parameters sheet for any convergence block.

The default diagnostic level within Aspen Plus is 4. At a Convergence Diagnostics Level of 4, a message is created in the Control Panel every time the convergence block executes. This message contains the following information:

- Convergence block
- Convergence method
- Iteration number
- What the convergence is trying to converge
- Number of unconverged variables
- Maximum error/tolerance for that iteration of the convergence block

Messages in the history file are similar, but not identical.

At a Convergence Diagnostics Level of 5, Aspen Plus creates a table of convergence information in the Control Panel for all unconverged variables.

For example:

```
 > Loop C-1      Method: BROYDEN      Iteration    1
  Converging tear streams: 4
  Converging specs: H2RATE
                            NEW X        G(X)         X           ERR/TOL
      TOTAL MOLEFLOW  (1) 0.135448E-01 0.135448E-01 0.000000E+00  10000.0
      N2 MOLEFLOW     (2) 0.188997E-03 0.188997E-03 0.000000E+00  10000.0
      C1 MOLEFLOW     (2) 0.755987E-03 0.755987E-03 0.000000E+00  10000.0
      BZ MOLEFLOW     (2) 0.314995E-03 0.314995E-03 0.000000E+00  10000.0
      CH MOLEFLOW     (2) 0.122848E-01 0.122848E-01 0.000000E+00  10000.0
      PRESSURE        (2) 0.217185E-01 0.217185E-01 0.100000E+36 0.100000E+07
      MASS ENTHALPY   (2)-0.137111E-01-0.137111E-01 0.100000E+36 0.100000E+07
      TOTAL MOLEFL    (3) 0.377994E-01 0.000000E+00 0.377994E-01 -375.000
  8 vars not converged, Max Err/Tol   0.17679E+05
```

The value in parentheses indicates the type of variable:

Variable Type	Description
1	Tear stream variable which is not updated by the convergence algorithm
2	Tear stream variable which is updated by the convergence method
3	Design specification manipulated variable. Updated by the algorithm
4	Fortran Tear Variable. Updated by the algorithm

New X is the value for the variable for the next iteration. X is the value of the variable for the previous iteration. G(X) is the calculated value for the variable at the end of the previous iteration. When a variable is converged, X and G(X) should differ by less than the tolerance. All values are in SI units.

Setting the Convergence Diagnostics level to 6 or higher does not change the amount of information reported in the Control Panel. However, it will affect the amount of information reported in the history file, depending on the convergence method in use.

Strategies for Flowsheet Convergence

Often a flowsheet can be converged without changing any convergence parameters.

Some general guidelines are:

- Start small. Make sure that individual blocks and elements of a flowsheet behave as expected, before slowly combining them into a larger simulation. A sensitivity block is useful for determining the results of other blocks under a range of conditions.
- Start with the simplest blocks possible. For example, converge the flowsheet with a simple HeatX before switching it to a rigorous HeatX.
- Give good initial guesses. Make sure the flowsheet starts converging from a reasonable point. Aspen Plus gives tear streams a default value of zero, which can cause problems. If possible, select a tear stream that remains relatively constant.
- Check physical properties. Make sure they are calculated correctly in the entire operating range of the simulation.
- Know how your flowsheet responds. Check the behavior of blocks and design specifications using sensitivity analysis. Look for discontinuities and flat regions that could cause convergence difficulties.
- Check for correctness, variable accessing, spelling, and unit specifications. When accessing real variables, make sure your variable names do not begin with I-N.

Tear Convergence Suggestions

This table shows the possible causes and solutions of tear stream convergence problems.

Diagnosing Tear Stream Convergence

If plot of Err/Tol vs. Iteration number shows	**A possible cause is**	**To correct the problem**
Steady convergence	—	Increase Maxit above 30 on the Conv Options or Convergence block Parameters sheet.
Steady but slow convergence	Component build-up	Check outlet streams from recycle loop to confirm that all components have a way to leave the system. If there is not, the problem may not be feasible from an engineering point of view. (That is, there may not be a steady state solution.)
	—	Allow for larger acceleration steps. For Wegstein, set Lower bound of the Wegstein acceleration parameter = -20 on the ConvOptions Wegstein sheet, or on the Convergence block Wegstein Input Parameters sheet. If this change speeds convergence, try lower bound = -50.
Oscillating convergence	—	For Wegstein, set upper bound to .5 to dampen the oscillations.
If plot of Err/Tol vs. Iteration number shows	A possible cause is	To correct the problem
Err/Tol down to a threshold level, but no further	Nested loops, and the convergence tolerance of the inner loops is too loose	Do one of the following: • Set a tighter tolerance for the blocks and convergence blocks in the inner loop, using the Tolerance field for these blocks. Block tolerance can be changed globally on the Setup SimulationOptions Flash Convergence sheet or locally on the block's Flash Options sheet. Convergence block tolerances can be changed globally on the Conv Options sheet for that method or locally on the convergence block's Parameter sheet. • Relax the tolerance for the outside loop. • Converge the inside and outside loops simultaneously, using the Broyden or Newton method. Use the Design Spec Nesting field on the ConvOptions Defaults Sequencing sheet.
Broyden or Newton failing to converge	—	Increase the value of Wait to 4 (on the Convergence ConvOptions sheet or Convergence block Parameters sheet). If both tear streams and design-specs are specified in the convergence block, solve only tear streams first by specifying Tear Tolerance or Tear Tolerance Ratio. Click the Advanced Parameters button on the Parameters sheet of the convergence block. Switch to the Wegstein method.

Some other general strategies for tear stream convergence are:

- Provide a good initial guess for the Tear stream on the Stream form. For more information on specifying streams, see Chapter 9.
- Select a Tear stream that will not vary a great deal. For example, the outlet stream of a Heater block is generally a better choice for a tear stream than the outlet stream from a Reactor block.
- Disconnect the recycle stream to get a good initial estimate and to examine the sensitivity.
- Try to simplify the problem. It may be possible to do one or more of the following to reduce the complexity of the problem:
  - Add a Mixer block to reduce the number of tear streams
  - Replace a HeatX block with an MHeatX to reduce the number of tear streams
  - Define and use a Component Group to reduce the number of variables
  - Choose a Tear stream that has fewer components present
  - Choose a Tear stream from a block that sets an outlet temperature
- Reinitialize the simulation. Try to converge the simulation using a Wegstein acceleration parameter equal to 0 (set the upper bound and lower bound to 0). This is equivalent to direct substitution. Look for a continuing buildup of one or more components as the iterations proceed.
- Try using a different convergence method such as Broyden or Newton rather than the default Wegstein method.
- Confirm that the sequence for the simulation (either Aspen Plus defined or user defined) is reasonable. See Specifying the Calculation Sequence, this chapter.

Design Specification Convergence Suggestions

This table shows the possible causes and solutions of Design Specification convergence problems.

Diagnosing Design Specification Convergence

If plot of Err/Tol vs. Iteration number shows	A possible cause is	To correct the problem
Steady convergence	—	Increase Maxit above 30 on the appropriate Conv Options or Convergence block Parameters sheet.
Err/Tol not changing	Spec function insensitive to manipulated variable	1. Check if the formulation of the spec function is correct. 2. Check if the correct manipulated variable is being used. 3. Use Sensitivity study to determine the effect of the manipulated variable on the spec function.
	Spec function flat over some range of the manipulated variable	For the Secant method, select Bracket=Yes on the Conv Options or Convergence block Parameters sheet, to use interval-halving method.

Continued

If plot of Err/Tol vs. Iteration number shows	A possible cause is	To correct the problem
Err/Tol down to a threshold level, but no further	Nested loops, and the convergence tolerance of the inner loops is too loose	Do one of the following: • Set a tighter tolerance for the blocks and convergence blocks in the inner loop, using the Tolerance field for these blocks. • Relax the tolerance for the outside loop. • Converge the inside and outside loops simultaneously, using the Broyden or Newton method. Use the Design Spec Nesting field on the ConvOptions Defaults Sequencing sheet.
Converged to variable bound	Non-monotonic Spec function	1. For the Secant method, select Bracket=Check bounds on the Conv Options or Convergence block Parameters sheet, to use interval-halving method. 2. Use Sensitivity study to determine the effect of the manipulated variable on the spec function. Adjust the bounds on the manipulated variable, or choose a better initial guess.

Some other general strategies for Design Specification convergence are:

- Formulate specifications to avoid discontinuities.
- Formulate specifications to reduce non-linearity with respect to design variables. For example, set a specification on the log of a concentration when it is near zero.
- Make sure the limits are reasonable. Try to avoid limits spanning more than one order of magnitude.
- Confirm the existence of a solution by replacing a Design specification with a Sensitivity block.
- Make sure the tolerance is reasonable, especially when compared with the tolerance of blocks inside the Design specification convergence block.

For more information on design specifications, see Chapter 21.

Fortran Block Convergence Suggestions

Some other general strategies for Fortran Blocks convergence are:

- Avoid iterative loops causing hidden mass balance problems. The sequencing algorithm can detect and converge Fortran tear variables, if the Fortran block is sequenced with Read and Write variables and if Tear Fortran Write Variables is checked on the ConvOptions Defaults Sequencing sheet. The Fortran tear variables are then solved along with the tear streams.
- Check the correctness of the Fortran statements in the Fortran block.
- Variables beginning with the letters I through N should be integer variables, if they have not been declared otherwise.

- Increase the diagnostics to check the value of variables used in the calculations. Click the Diagnostics button on the Fortran Sequencing sheet. On the Diagnostics dialog box, raise the level for Fortran Defined Variables to 5 or 6. This will print out the value of the accessed variables.
- Add write statements to your Fortran block to print out the value of intermediate variables.
- If using Read and Write variables to determine the sequence, make sure that all the variables are listed.

For more information on Fortran Blocks, see Chapter 19.

Resolving Sequence and Convergence Problems

Use the following strategy to resolve sequence or convergence problems:

1. Run the simulation using the default sequence generated by Aspen Plus.
2. Examine simulation results, looking for skipped and unconverged unit operation blocks. Check the Control Panel and results sheets for blocks that did not complete normally, had errors, or had unexpected results that might affect recycle convergence. See Checking Convergence Results, this chapter, for more information.

   Some common reasons for these problems are:

Problem	Action
Incorrect block specifications	Correct them.
Feed conditions too far off	Provide better estimates for tear streams and/or design variables.
Convergence specifications	Try different specifications, different algorithm options, or increase the number of iterations.
Algorithm options	Change options.
Not enough iterations	Increase number of iterations.

   If you make any corrections, go to step 9.

3. Check whether tolerance needs adjustment. If the maximum error/tol for convergence blocks reduces to around 10 quickly, but fluctuates after that, tolerance adjustments may be necessary. For more information, see the Sequencing Example.

   Another way to correct tolerance problems is to converge multiple design specifications with a Broyden or Newton convergence block.

4. If Wegstein convergence blocks converge slowly, try some Wegstein parameters, such as Wait=4, Consecutive Direct Substitution Steps=4, Lower Bound=-50. Providing better estimates for tear streams would also help.

5. If tear stream convergence blocks oscillate, try using the Direct method for convergence. If the problem persists, examine the flowsheet to determine if every component has an outlet. The oscillation of a tear stream loop could also be caused by the non-convergence of design specification loops inside the tear stream loop; check for this next, if oscillation persists. If oscillation stops, try the acceleration technique described in step 4.
6. Examine the Spec Summary and check for non-converged design specifications. Some common reasons for a design specification that does not converge are:

Design Specification Problem	Action
Not reachable within bounds on variable	Accept the solution or relax the bounds.
Not sensitive to manipulated variable	Select a different manipulated variable to meet the design specification or delete the design specification.
Insensitive to manipulated variable in a certain range	Provide a better initial guess, refine the bounds, and/or enable the Bracket option of the Secant convergence method.
Not sensitive to the manipulated variable, because the design specification loop is not nested properly	See Sequencing Example, this chapter. If it is necessary to alter the calculation sequence, see step 7.

7. Alter the calculation sequence, if necessary, using one of the following options. (This step requires a good understanding of the process you are simulating and is intended for advanced users only):

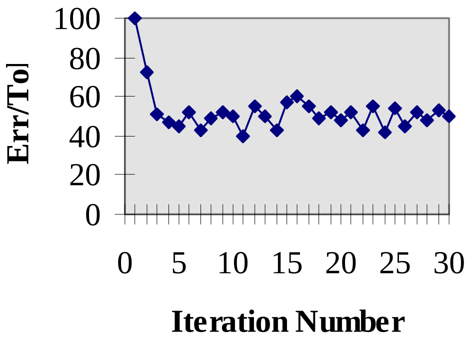
If you want to	Specify
Make one or more design specification loops the outermost loops	These loops on the ConvOrder Specifications sheet (See Specifying Convergence Order, this chapter)
Alter the nesting of a small section of the flowsheet	A partial sequence on the Sequence Specifications sheet (see Specifying the Calculation Sequence, this chapter)
Use specific tear streams	These streams on the Tear Specifications sheet (see Specifying Tear Streams, this chapter)

   There are other options on the ConvOptions Defaults Sequencing sheet that also affect the calculation sequence (see Convergence Options, this chapter).

8. If all convergence blocks are converged but the overall mass balance is not in balance, check Fortran blocks for possible errors. It is recommended that you use Read and Write Variables to sequence regular Fortran blocks, and use Execute to sequence initialization Fortran blocks.
9. If the flowsheet is modified, rerun the simulation and go back to step 2.

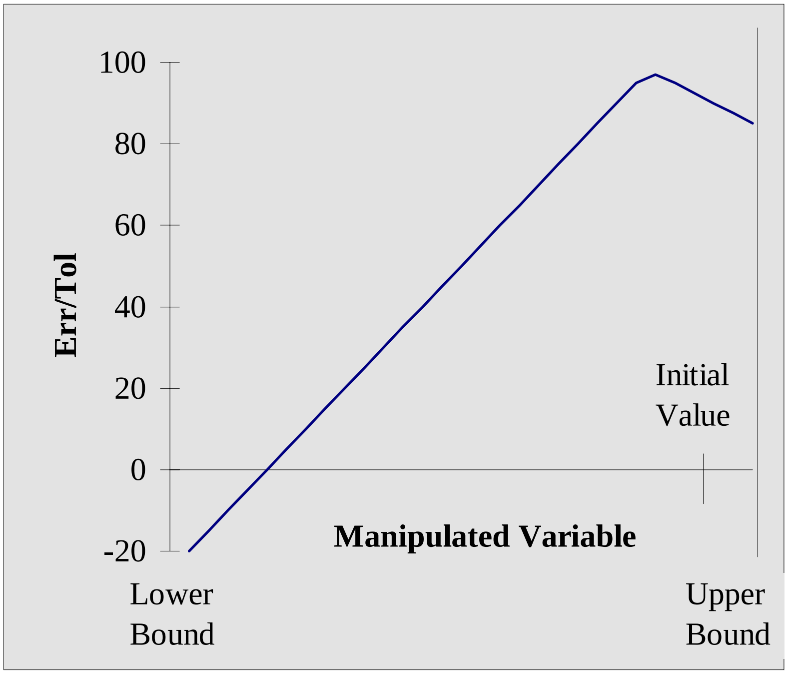
Example of Err/Tol Going Down to a Threshold Value

After about 8 recycle convergence iterations, the Err/Tol value goes down to a threshold value, but not lower. This recycle is nested outside of an inner design specification loop. Set a tighter tolerance for the inner loop.



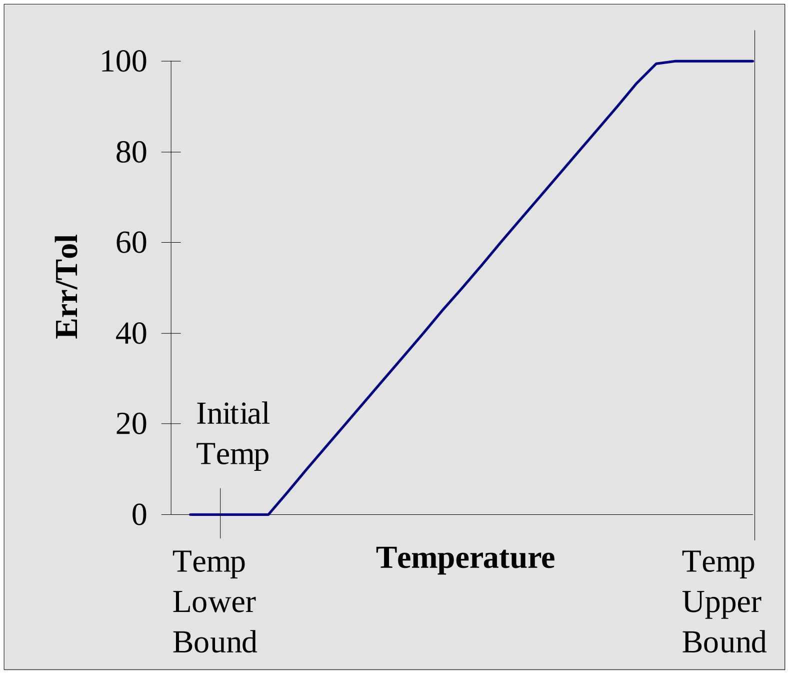
Example of Manipulated Variable Moving to a Bound

This design specification function is non-monotonic. Depending on the initial value of the manipulated variable, the convergence algorithm may move the manipulated variable to the upper bound, even though a solution exists within the bounds. Specify Check Bounds in the Bracket field on the Convergence ConvOptions Methods Secant sheet or Secant Input Parameters sheet. Ensure that the secant algorithm checks both bounds, to try to bracket the solution.



Example of Err/Tol Value Not Changing

The Err/Tol value does not change for a design specification, where the temperature of a reactor is being manipulated to control the conversion in the reactor. A sensitivity analysis shows that the specification function (conversion) is flat over some range of the manipulated variable. Specify Yes in the Bracket field on the Convergence ConvOptions Methods Secant sheet or Secant Input Parameters sheet for this design specification problem.



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18 Accessing Flowsheet Variables

You access or manipulate flowsheet variables when using the following capabilities:

- Design specifications
- Fortran blocks
- Optimization problems
- Data-Fit problems
- Sensitivity blocks
- Case study

This chapter describes:

- Accessing flowsheet variables
- Types of accessible flowsheet variables
- Choosing input and parameter variables
- The layout (or structure) of the vector variable types
- Examples of how the accessed variables are used in Fortran statements

Accessing Flowsheet Variables

When you run a simulation in Aspen Plus, you often need to record or modify the value of quantities in the simulation, such as the temperature of a flash block or the mass flow of a stream. References to flowsheet quantities are made by “accessing” these variables.

For example, to study the effect of a column reflux ratio on the mole fraction of a component in the distillate, two flowsheet quantities (variables) would need to be accessed: the reflux ratio of the column and the mole fraction of the component in the distillate. Several features in Aspen Plus require you to access variables, such as design specifications, Fortran blocks, optimization problems, data-fit problems, and sensitivity blocks.

Most accessed variables have a user-specified name associated. For example, you could associate the name “PRES” with a variable that points to the pressure in a Flash2 block. However, variables that are to be varied by a design-spec, a sensitivity block, or optimization do not have a name associated.

There are two kinds of variables in a simulation:

Type of Variable	Information
Those which you enter	You can manipulate directly any variables that you enter. These variables may be either read or written.
Those calculated by Aspen Plus	These variables should not be overwritten or varied directly, as this would lead to inconsistent results. These variables should only be read.

Accessed variables can be either scalar or vector. An example of a scalar variable is the pressure for a specific stage in a RadFrac block. The pressure profile for a column is an example of a vector variable. For more information, see Types of Accessed Flowsheet Variables, this chapter.

It is important to make sure the correct variable is accessed. Look at the prompt at the bottom of the form when you select a variable from a drop-down list.

For example, when you select the block variable for a Flash2 or a Heater called PDROP, the prompt tells you that this is the pressure drop for the heating or cooling curve (not the pressure drop for the block). When you select the variable PRES, the prompt tells you that this variable is the pressure specification for the block; the value will be negative if pressure drop was input.

Types of Accessed Flowsheet Variables

Values for accessed scalar variables are in the units specified in the Units field (on the Data Browser toolbar). For example, you might define a variable as a stream temperature on the Design Spec Define sheet. If the Units field for the sheet says ENG, the accessed temperature value is in degrees Fahrenheit. Vector variables are in SI units, regardless of the Units specified.

There is only one set of units for an object. All accessed variables (both defined and varied) for an object are in the same set of units.

You can access flowsheet variables for these variable types:

- Block variables
- Stream variables
- Other variables
- Property parameters

Block Variables

Variable type	Description
Block-Var	Unit operation block variable
Block-Vec	Unit operation block vector

Stream Variables

Variable type	Description
Stream-Var†	Non-component-dependent stream variable
Stream-Vec	Stream vector. See Accessing Stream and Substream Vectors
Substream-Vec	Substream variable. See Accessing Stream and Substream Vectors
Mole-Flow	Component mole flow in a stream
Mole-Frac††	Component mole fraction in a stream
Mass-Flow	Component mass flow in a stream
Mass-Frac††	Component mass fraction in a stream
Stdvol-Flow	Component standard liquid volume flow in a stream
Stdvol-Frac††	Component standard liquid volume fraction in a stream
Heat-Duty	Heat stream duty
Work-Power	Work stream power
Stream-Prop††	Stream property defined by a property set
Compattr-Var	Component attribute element
Compattr-Vec	Component attribute vector
PSD-VAR	Substream Particle Size Distribution (PSD) element
PSD-Vec	Substream Particle Size Distribution (PSD) vector

† ***These stream variables can be accessed only as results.You cannot change or set them.: MOLE-ENTHALPY, MASS-ENTHALPY, MOLE-ENTROPY, MASS-ENTROPY, MOLE-DENSITY, MASS-DENSITY, LFRAC***

†† ***Variables of this type can be accessed only as results. You cannot change or set them.***

Other Variables

Variable type	Description
Balance-Var	Balance block variable
Chem-Var	Chemistry variable
Presr-Var	Pressure relief variable
React-Var	Reactions variable
Parameter	User-defined parameter. See Using Parameter Variables

Property Parameters

Accessed property parameters are always in SI units.

Variable type	Description
Unary-Param	Scalar unary property parameter
Unary-Cor-El	Temperature-dependent unary property parameter coefficient element
Un-Cpr-Vec	Temperature-dependent unary property parameter coefficient vector. For more information, see Accessing Property Parameter Vectors
Bi-Param	Scalar binary property parameter
Bi-Cor-El	Temperature-dependent binary property parameter coefficient element
Bi-Cor-Vec	Temperature-dependent binary property parameter coefficient vector.
NC-Param	Nonconventional component parameter

Variable Definition Dialog Box

When completing a Define sheet, such as on a Fortran, Design specification or Sensitivity form, specify the variables on the Variable Definition dialog box. The Define sheet shows a concise summary of all the accessed variables, but you cannot modify the variables on the Define sheet.

When on any Define Sheet:

1. To create a new variable, click the New button.

   – or –

   To edit an existing variable, select a variable and click the Edit button.

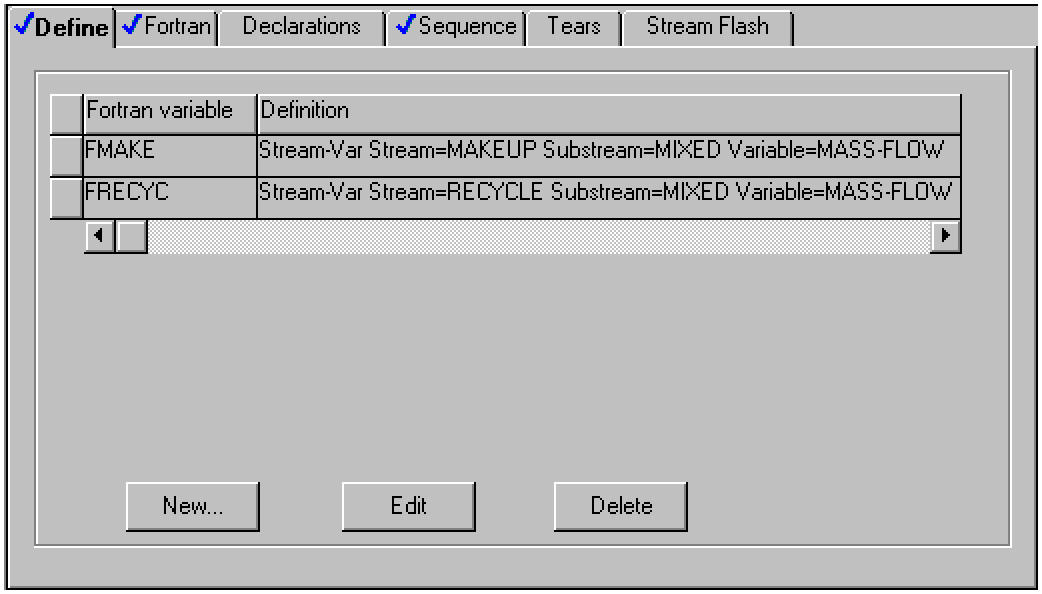
2. Type the name of the variable in the Variable Name field.
3. In the Category frame, use the option button to select the variable category.
4. In the Reference frame, select the variable type from the list in the Type field.

   Aspen Plus displays the other fields necessary to complete the variable definition.
5. Click Close to return to the Define sheet.

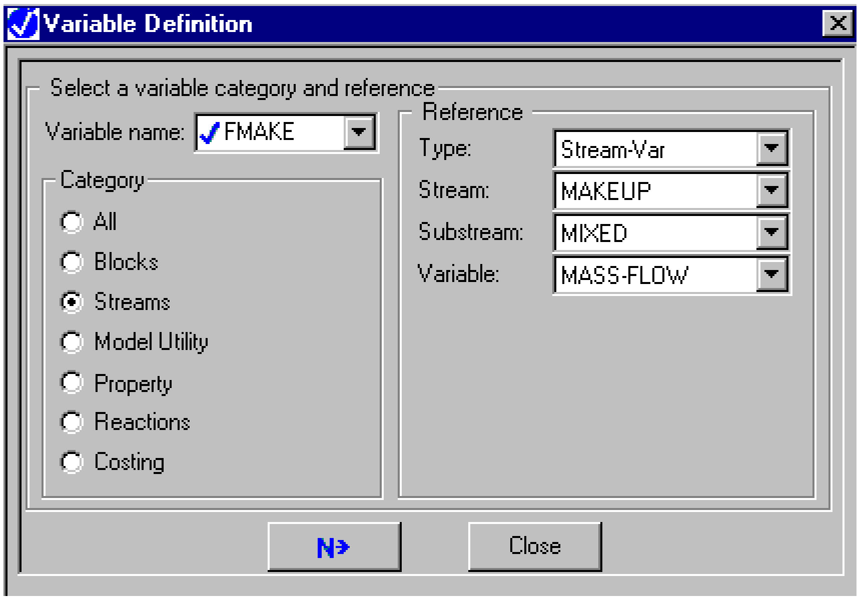
Example for Calculating Make-up Flow Rate

The mass flow rate of a make-up stream (MAKEUP) is determined by the difference between the mass flow rate of the recycle stream (RECYCLE) and 120 lb/hr, using a Fortran block. Aspen Plus writes the make-up flow rate to the Control Panel.

On the Fortran Define sheet, Fortran variables FMAKE and FRECYC are defined for the two stream mass flow rates. The Variable Definition dialog box is used to define the variables.



Fortran variable	Definition
FMAKE	Stream-Var Stream=MAKEUP Substream=MIXED Variable=MASS-FLOW
FRECYC	Stream-Var Stream=RECYCLE Substream=MIXED Variable=MASS-FLOW



Variable name: FMAKE

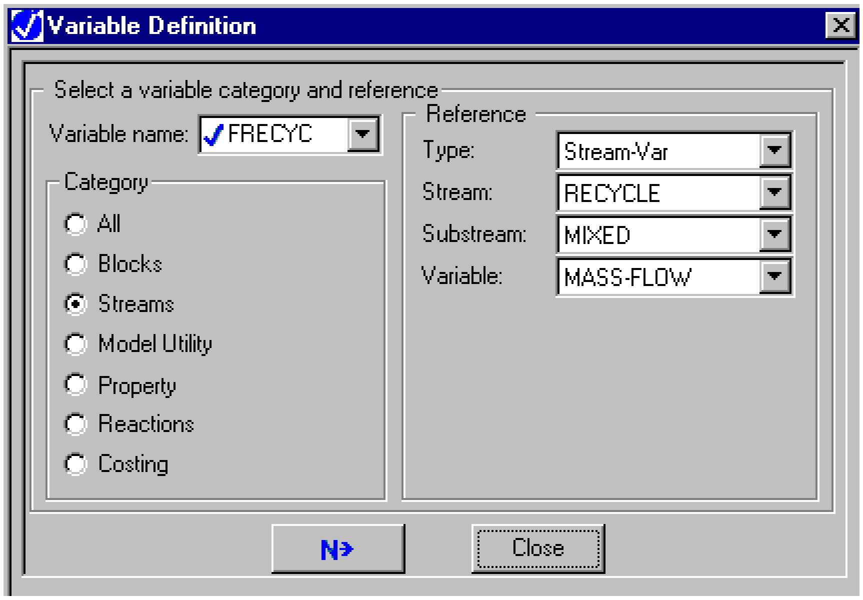
● Streams

Type: Stream-Var

Stream: MAKEUP

Substream: MIXED

Variable: MASS-FLOW



Variable name: FRECYC

● Streams

Type: Stream-Var

Stream: RECYCLE

Substream: MIXED

Variable: MASS-FLOW

On the Fortran Fortran sheet, these Fortran statements are included:

```
F     FMAKE=120.0-FRECYC
C     If no makeup is required, set
C     the makeup to a small value
C     to avoid losing the makeup
C     stream composition
      IF(FMAKE.LE.0.0) FMAKE=0.0001
      WRITE(NTERM,10) FMAKE
  10  FORMAT(1X,'MAKEUP FLOW RATE=', F10.2)
```

Choosing Input or Results Variables

It is sometimes important to distinguish between input and results when accessing:

- Block variables
- Pressure relief variables

For example, suppose you are sampling the calculated duty of a Heater block that has temperature and vapor fraction specified. You must access the results variable QCALC, not the input variable DUTY. DUTY will not have a value.

To determine whether a variable is an input or results variable:

1. In the Variable Definition dialog box where you are accessing the variable, click the arrow in the Variable field, and select the variable from the list.
2. Check the prompt. If the prompt begins with Calculated, the variable is a results variable. Otherwise it is an input variable.

Guidelines for Choosing Input or Results Variables

Follow these guidelines for choosing input or results variables:

- Choose input variables when setting or manipulating input specifications.
- Choose results variables for use in design specification expressions, optimization objective functions, constraint expressions, and sensitivity tabulations.
- See Chapter 19 for special considerations when accessing variables in a Data-Fit block.
- If a result is available in an outlet stream of a block, access the stream variable. For example, to access the temperature calculated by a Heater block, access the temperature of the outlet stream.
- If a result is not available in an outlet stream of a block, choose a block variable with a prompt that begins with Calculated. For example, the prompt for the variable QCALC (the duty calculated by a Heater block) is Calculated heat duty.
- MASS-FRAC, MOLE-FRAC and STDVOL-FRAC are results variables and cannot be changed.

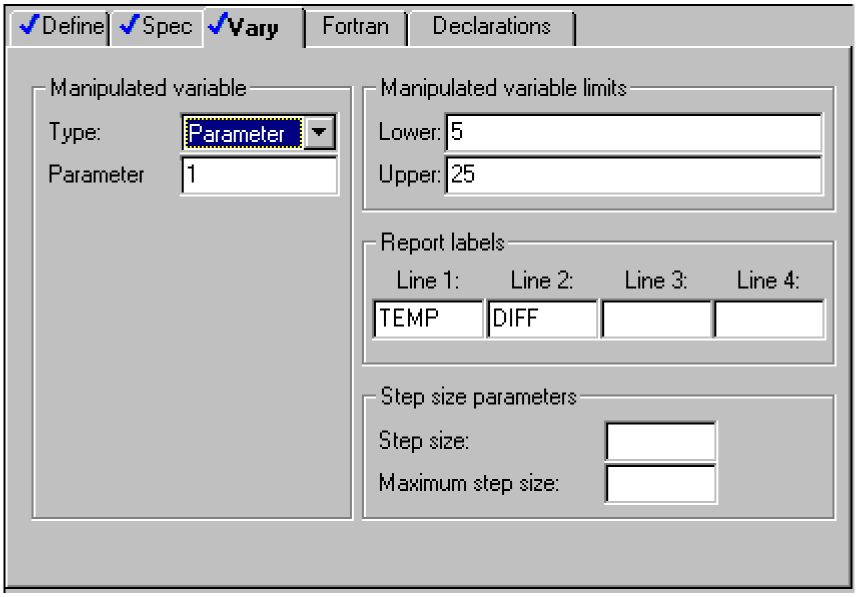
Using Parameter Variables

A parameter variable is a user-defined global variable you can use for temporary storage of quantities not defined in Aspen Plus. For example, the temperature difference between two blocks can be a parameter variable. You identify parameter variables by variable number. There can be any number of parameter variables in a simulation.

Example of Using a Parameter Variable for Temperature Difference

A design specification manipulates a user-defined variable (Parameter 1), which represents the temperature difference between two heaters. A Fortran block retrieves the parameter (DELT) and the temperature of the first heater (T1), and uses these variables to set the temperature of the second heater (T2). The Variable Definition dialog box is used to define the variables on the Fortran Define sheet.

On the Design Spec form:



Type: Parameter

Parameter 1

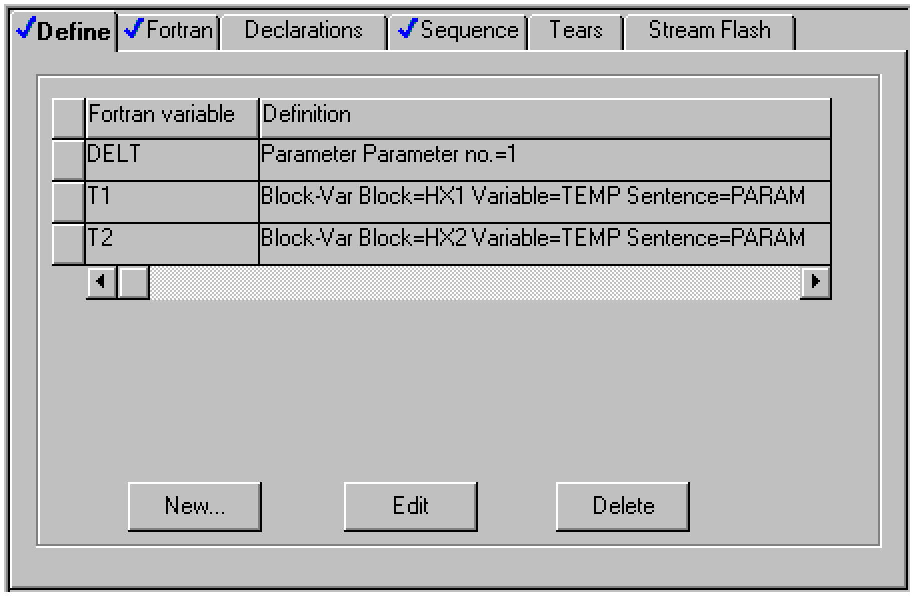
Lower: 5

Upper: 25

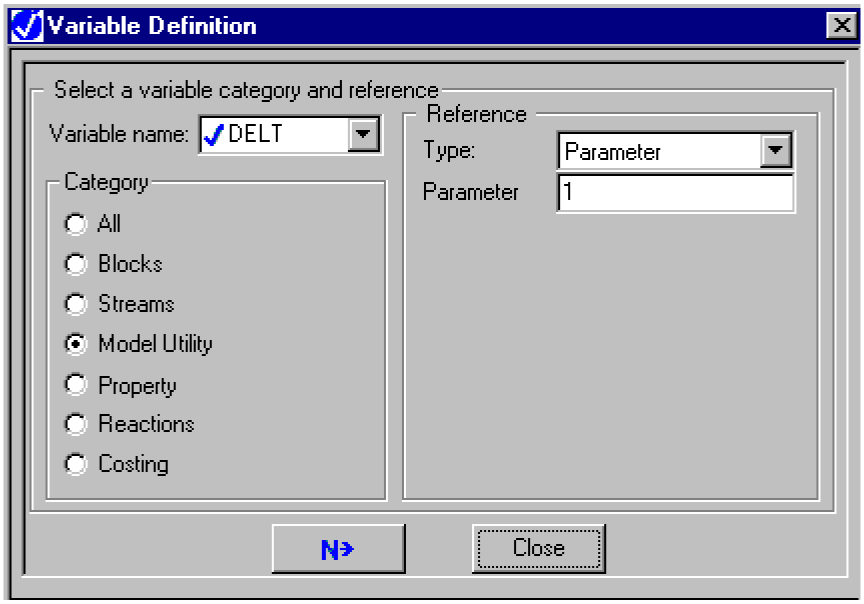
Line 1: TEMP

Line 2: DIFF

On the Fortran form:



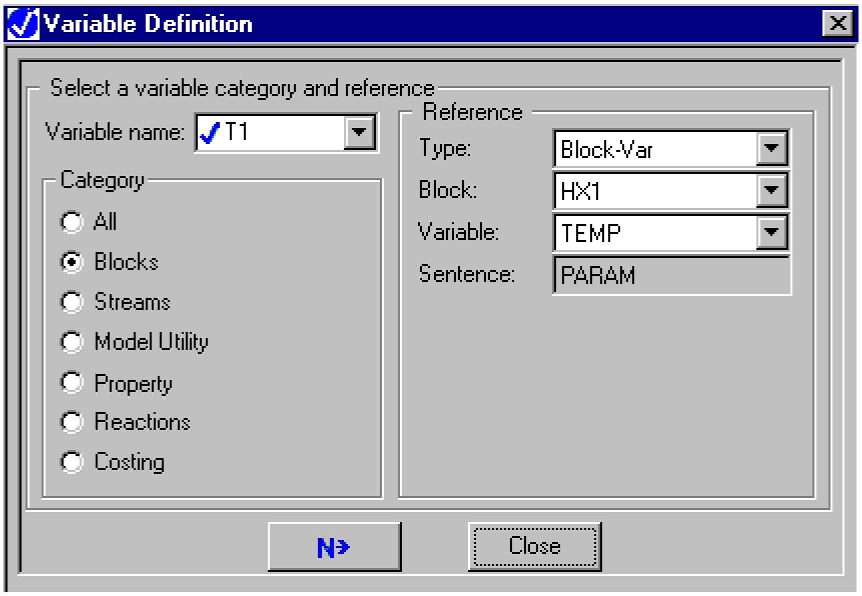
Fortran variable	Definition
DELT	Parameter Parameter no.=1
T1	Block-Var Block=HX1 Variable=TEMP Sentence=PARAM
T2	Block-Var Block=HX2 Variable=TEMP Sentence=PARAM



Variable name: DELT

Type: Parameter

Parameter 1

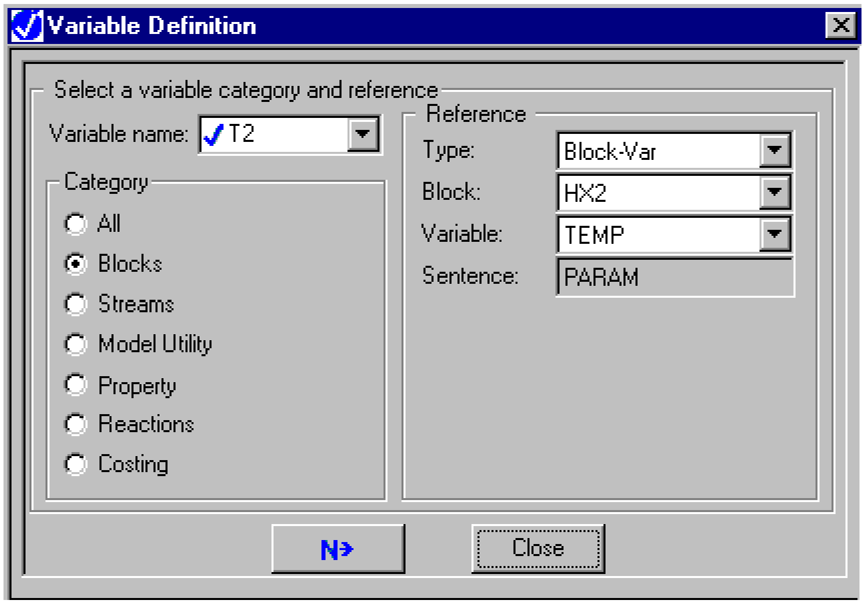

Variable Definition

Select a variable category and reference

Variable name: T1

Category
○ All
● Blocks
○ Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

Reference
Type: Block-Var
Block: HX1
Variable: TEMP
Sentence: PARAM

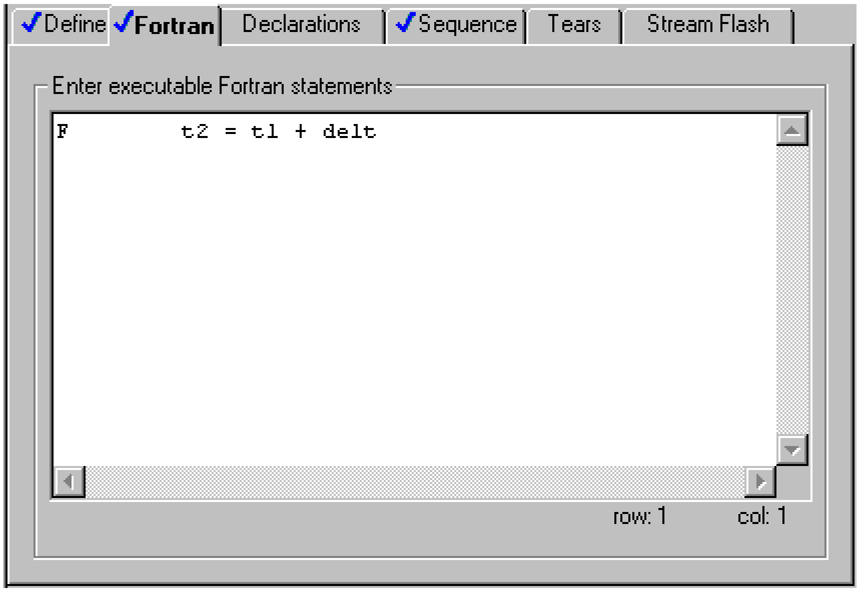

Variable Definition

Select a variable category and reference

Variable name: T2

Category
○ All
● Blocks
○ Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

Reference
Type: Block-Var
Block: HX2
Variable: TEMP
Sentence: PARAM



```
F        t2 = t1 + delt
```

Accessing Vectors

You can use the vector variable types to access an entire block profile, stream or substream at once. Aspen Plus interprets the Fortran variable you assign to the vector as an array variable. You do not need to dimension it.

Vector Variables

Variable type	Description
Block-Vec	Unit operation block vector (see Accessing Block Vectors, this chapter)
Stream-Vec	Stream vector (see Accessing Stream and Substream Vectors, this chapter)
Substream-Vec	Substream variable (see Accessing Stream and Substream Vectors, this chapter)
Compattr-Vec	Component attribute vector (see Component Attributes and PSD, this chapter)
PSD-Vec	Substream Particle Size Distribution (PSD) vector (see Component Attributes and PSD, this chapter)
Un-Cor-Vec	Temperature-dependent unary property parameter vector (see Accessing Property Parameter Vectors, this chapter)
Bi-Cor-Vec	Temperature-dependent binary property parameter vector (see Accessing Property Parameter Vectors, this chapter)

Aspen Plus generates a variable by adding the letter L to the beginning of the Fortran variable name which you assign to the vector. The value of this variable is the length of the vector. You can use the variable in Fortran statements, but you cannot change its value.

Accessing Stream and Substream Vectors

You can use the Stream-Vec and Substrm-Vec variable types to access an entire stream or substream at once. Aspen Plus interprets the Fortran variable you assign to the stream as an array variable. You do not need to dimension it.

A stream vector contains all the substream vectors for that stream class. The order of the substreams is defined on the Define Stream Class dialog box (click the Define Stream Class button on the Setup StreamClass Flowsheet sheet).

The variables in a stream or substream vector are always in SI units.

Substream MIXED and Stream Class CONVEN

This is the layout of the substream vector for substream MIXED and for Stream-Vec, when accessing the default stream class CONVEN:

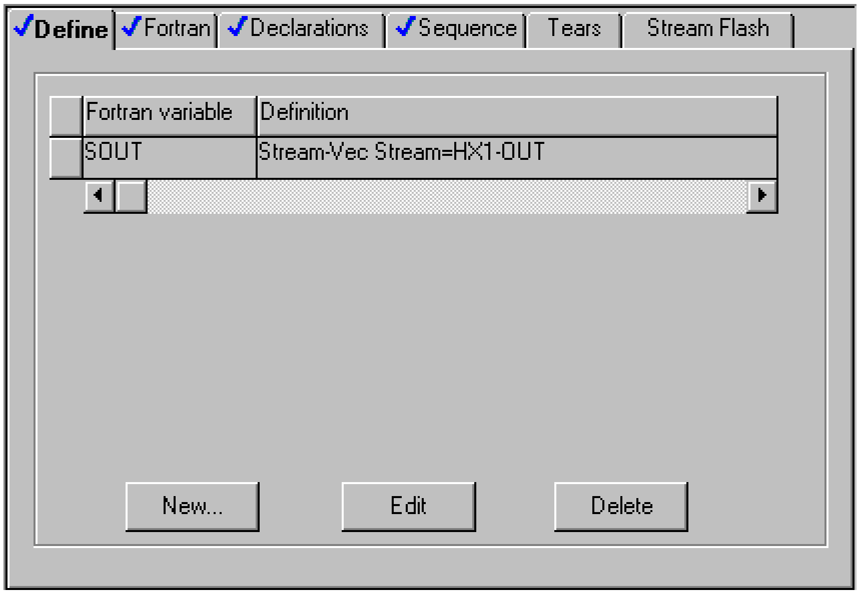
Array Index	Description
1, . . . , NCC	Component mole flows (kg-moles/sec)
NCC + 1	Total mole flow (kg-moles/sec)
NCC + 2	Temperature (K)
NCC + 3	Pressure (N/m^2)
NCC + 4	Mass enthalpy (J/kg)
NCC + 5	Molar vapor fraction
NCC + 6	Molar liquid fraction
NCC + 7	Mass entropy (J/kg-K)
NCC + 8	Mass density (kg/m^3)
NCC + 9	Molecular weight (kg/kg-mole)

NCC is the number of conventional components specified on the Components Specifications Selection sheet. The order of the component mole flows is the same as the order of components on that sheet. All values are in SI units, regardless of the Units specification on the Define sheet.

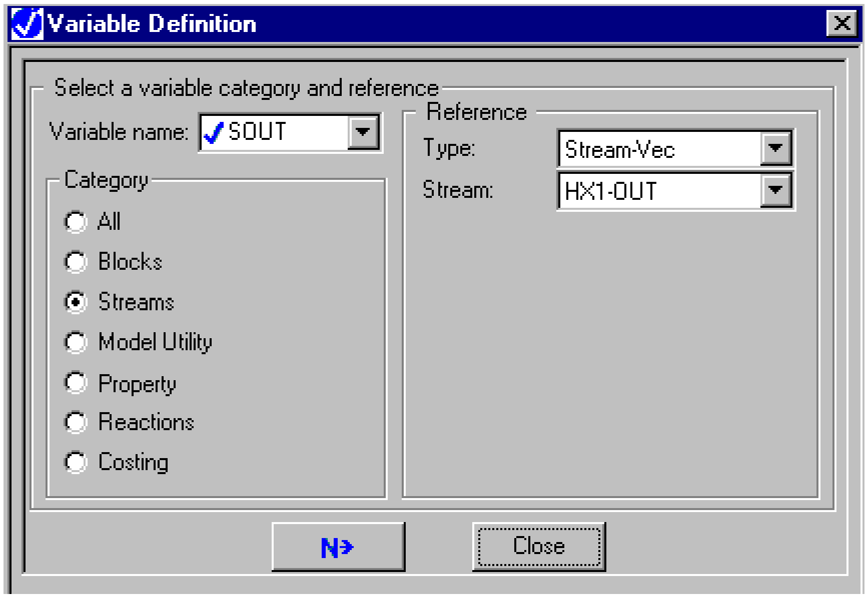
Aspen Plus generates a variable by adding the letter L to the beginning of the Fortran variable name, which you assign to the substream or stream vector. The value of this variable is the length of the vector (NCC + 9). You can use the variable in Fortran statements, but you cannot change its value.

Example for Accessing a Stream Vector

A Fortran block is used to write the mole fractions of stream HX1-OUT to the terminal. On the Define sheet of the Fortran block, Fortran variable SOUT, of the type Stram-Vec, is defined.



Fortran variable	Definition
SOUT	Stream-Vec Stream=HX1-OUT



Variable name: SOUT

○ All
○ Blocks
● Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

Type: Stream-Vec

Stream: HX1-OUT

On the Fortran Fortran sheet, these Fortran statements are included:

```
      NCOMP=LSOUT-9
      WRITE(NTERM,30)
      DO 10 I=1, NCOMP
      X(I)=SOUT(I)/SOUT(NCOMP+1)
      WRITE(NTERM, 20) I, X(I)
10    CONTINUE
20    FORMAT (10X, I3, 2X, F10.4)

30    FORMAT ('STREAM HX1-OUT MOLE FRACTIONS')
```

On the Fortran Declarations sheet, the following statement allows for up to 20 components:

```
      DIMENSION X(29)
```

Substream CISOLID

The layout of a substream vector for a CISOLID substream is the same as for a MIXED substream, with one exception. If the CISOLID substream has a PSD, an array of values for the PSD is appended to the vector. NCC is the number of conventional components. Space for all conventional components is reserved in both the MIXED and CISOLID substreams. The component order is the same as on the Components Specifications Selection sheet. All values are in SI units, regardless of the Units specification.

In the following table, n represents the number of intervals in the particle size distribution. For CISOLID substreams, vapor and liquid fractions have the value 0.0. This is the layout of a substream vector for a CISOLID substream:

Array Index	Description
1, . . . , NCC	Conventional component mole flows (kg-moles/sec)
NCC + 1	Total mole flow (kg-moles/sec)
NCC + 2	Temperature (K)
NCC + 3	Pressure (N/m^2)
NCC + 4	Mass enthalpy (J/kg)
NCC + 5	Molar vapor fraction (0.0)
NCC + 6	Molar liquid fraction (0.0)
NCC + 7	Mass entropy (J/kg-K)
NCC + 8	Mass density (kg/m^3)
NCC + 9	Molecular weight (kg/kg-mole)
NCC + 10 . . . . . . NCC + 9 + n	frac . . . frac$_n$ } PSD values (if a PSD attribute is defined for the substream)

Aspen Plus generates a variable by adding the letter L to the beginning of the Fortran variable name which you assigned to the substream or stream vector. The value of this variable is the length of the vector (NCC + 9 + n). You can use the variable in Fortran statements, but you cannot change its value.

Substream NC

A substream vector for an NC substream contains:

- Component flows
- Stream conditions
- Component attributes
- An array of values for the PSD (if the substream has a PSD)

NNCC is the number of nonconventional components.

The component order for	Is the same as on
Component flows	Components Specifications Selection sheet
Component attributes	Properties Advanced NC-Props Property Methods sheet

Attributes for each component appear in the order specified on the Properties Advanced NC-Props Property Methods sheet for that component. All values are in SI units, regardless of the units specification.

This is the layout of a substream vector for an NC substream:

Array Index	Description
1, . . . , NNCC	Component mass flows (kg/sec)
NNCC + 1	Total mass flow (kg/sec)
NNCC + 2	Temperature (K)
NNCC + 3	Pressure (N/m^2)
NNCC + 4	Mass enthalpy (J/kg)
NNCC + 5	Vapor fraction (0.0)
NNCC + 6	Liquid fraction (0.0)
NNCC + 7	Mass entropy (J/kg-K)
NNCC + 8	Mass density (kg/m^3)
NNCC + 9	1.0
NINCC + 10	$\left.\begin{matrix}\text{value}_1\\ .\\ .\\ .\\ \text{value}_k\end{matrix}\right\}$ Values for component attribute 1 of component 1 $\left.\begin{matrix}\text{value}_1\\ .\\ .\\ .\\ \text{value}_l\end{matrix}\right\}$ Values for component attribute 2 of component 1 $\left.\begin{matrix}\text{value}_1\\ .\\ .\\ .\\ \text{value}_m\end{matrix}\right\}$ Values for component attribute 1 of component 2 $\left.\begin{matrix}\text{frac}_1\\ .\\ .\\ .\\ \text{frac}\end{matrix}\right\}$ PSD values (if a PSD attribute is defined for the substream)

Component Attributes and PSD

You can use the Compattr-Vec and PSD-Vec variable types to access component attribute vectors and PSD vectors of streams. The layout of the vector is the list of elements for the attribute. See Substream CISOLID and Substream NC for the layout for substream PSD, in this chapter. See Chapter 6 for a description of the elements for each component attribute. You can also obtain information for the attribute from the Components Attr-Comps Selection sheet and Properties Advanced NC-Props Property Methods sheet.

Accessing Block Vectors

You can use the Block-Vec variable type to access column profiles for the following multi-stage separation models:

In this model	Variables depend on
RadFrac	Stage and composition
MultiFrac	Stage, section, and composition
Extract	Stage
PetroFrac	Stage, composition, and stripper number
RateFrac™	Segment, composition, and accumulator number
BatchFrac™	Stage, composition, and operation step
SCFrac	Section and composition

You can also use Block-Vec to access the following block result profiles:

- MHeatX zone analysis
- RBatch time profiles
- RPlug length profiles

Aspen Plus automatically:

- Interprets the Fortran variable you assign to the profile as an array variable
- Dimensions the variable

Aspen Plus generates a variable by adding the letter L to the beginning of the Fortran variable name which you assigned to the block vector. The value of this variable is the length of the array. You can use the variable in FORTRAN statements, but you cannot change its value.

The order of values in the Fortran array depends on which variable you select. Subsequent sections of this chapter describe the order for variables. All values are in SI units, regardless of the Units specifications on the Define sheet.

Variables Dependent on Stage Number or Segment Number

The layout for vector variables is dependent on stage, section or segment number follows.

Array Index	Value for
1	Stage or segment 1
2	Stage or segment 2
.	
.	
N	Last stage or segment

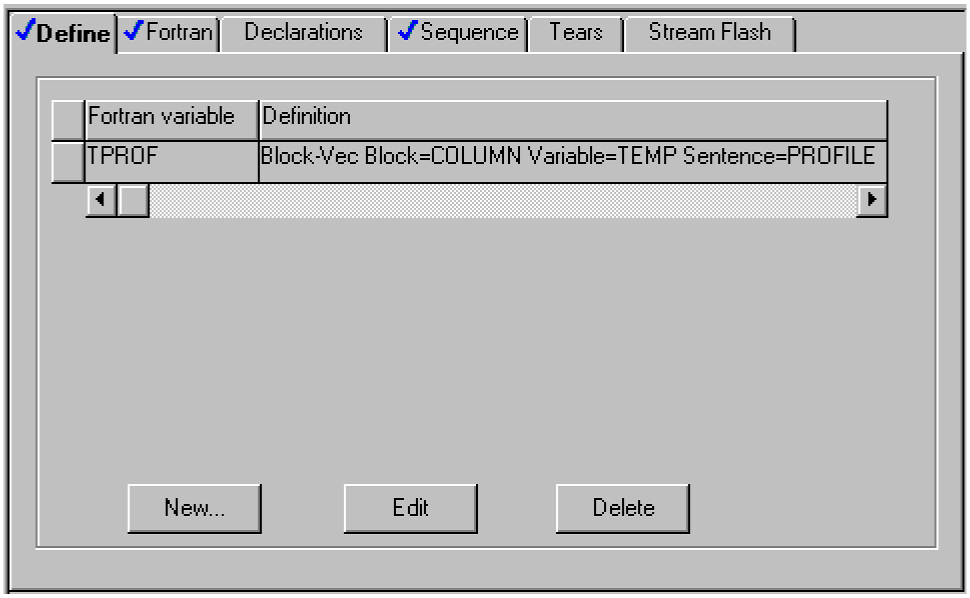
N denotes the number of stages or segments in the column.

Examples of variables dependent on stage number are temperature and flow profiles in RadFrac, MultiFrac Extract, PetroFrac, or BatchFrac. Examples of vector variables dependent on segment number are temperature and flow profiles for RateFrac.

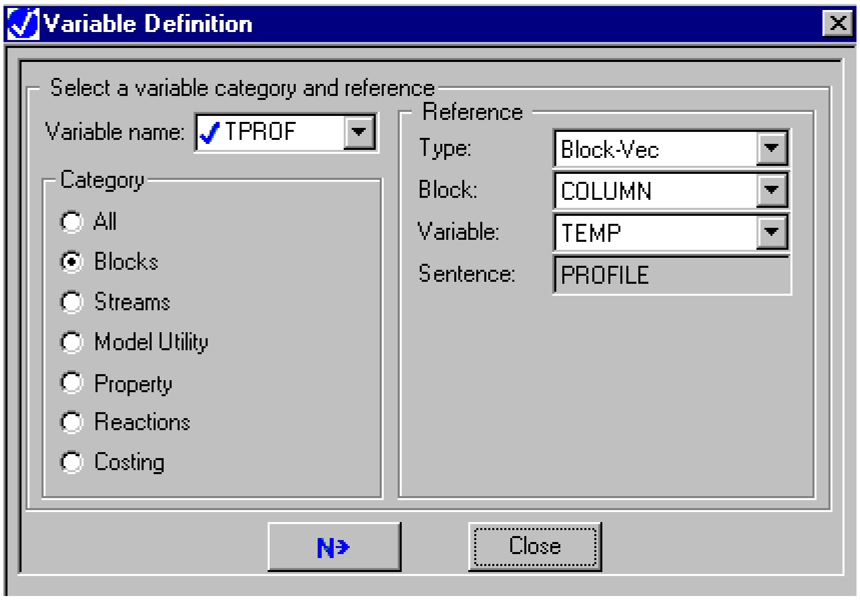
Example for Accessing a Temperature Profile

The temperature profile of a RadFrac block is written to the Control Panel, using a Fortran block.

On the Define sheet of the Fortran block, Fortran variable TPROF of the type Block-Vec is defined using the Variable Definition dialog box.



Fortran variable	Definition
TPROF	Block-Vec Block=COLUMN Variable=TEMP Sentence=PROFILE



Variable name: ✓ TPROF

Category
○ All
● Blocks
○ Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

Reference
Type: Block-Vec
Block: COLUMN
Variable: TEMP
Sentence: PROFILE

On the Fortran Fortran sheet, these Fortran statements are included:

```
   WRITE(NTERM,20)
C* LTPROF IS AUTOMATICALLY GENERATED BY Aspen Plus *
      DO 10 I = 1, LTPROF
      WRITE(NTERM,30) I, TPROF(I)
   10 CONTINUE
   20 FORMAT ('   *** TEMPERATURE PROFILE ***')
   30 FORMAT (10X, I3, 2X, F10.2)
```

Variables Dependent on Section Number

Examples of vector variables dependent on section number are fractionation index and duty results for SCfrac, and the sizing/rating results for trays and packings. The layout, where Nsec denotes the number of sections in the column, is:

Array Index	Value for
1	Section 1
2	Section 2
.	
.	
Nsec	Last section

Variables Dependent on Operation Step Number

Examples of vector variables dependent on operation step number are distillate and reflux ratio results for BatchFrac. The layout, where Nopstep denotes the number of operation steps, is:

Array Index	Value for
1	Operation step 1
2	Operation step 2
.	
.	
Nopstep	Last operation step

Variables Dependent on Component Number

Examples of vector variables dependent on component number are RadFrac thermosyphon reboiler compositions. The layout follows, where NCC denotes the number of components entered on the Components Specifications Selection sheet. The component order is the same as on that sheet.

Array Index	Value for
1	Component 1
2	Component 2
.	
.	
.	
NCC	Last component

Variables Dependent on Component Number and Stage or Segment Number

Examples of vector variables dependent on component number and stage number are liquid and vapor composition profiles in RadFrac, MultiFrac, Extract, PetroFrac, or BatchFrac. Examples of vector variables dependent on component number and segment number are liquid and vapor composition profiles for RateFrac. The values are stored as one-dimensional arrays. All component values for stage or segment 1 are at the beginning, followed by all of the component values for stage or segment 2, and so on. The number of components and the component order are the same as on the Components Specifications Selection sheet.

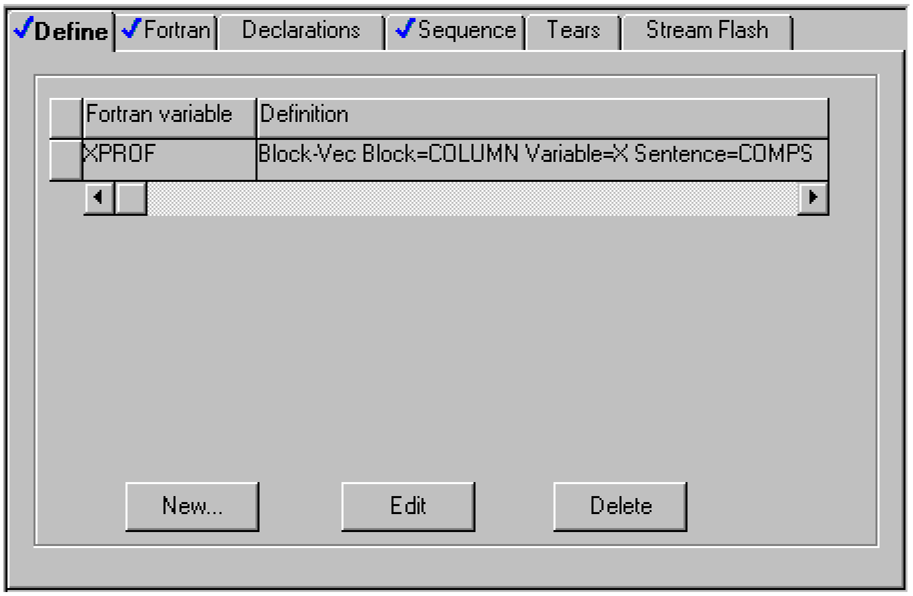
For a column with three components and five stages, the liquid composition profile is stored as follows:

Array Index	Value for
1	Component 1, stage or segment 1
2	Component 2, stage or segment 1
3	Component 3, stage or segment 1
4	Component 1, stage or segment 2
.	
.	
.	
15	Component 3, stage or segment 5

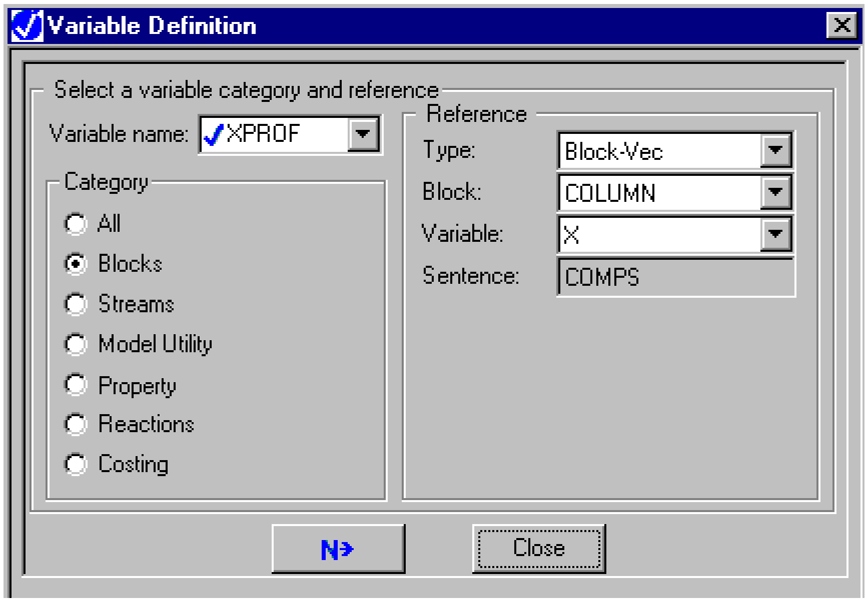
Example for Accessing a Mole Fraction Profile

The entire liquid mole fraction profile of a RadFrac column with three components is accessed. The value for the second component on the fifth stage is written to the Control Panel, using a Fortran block.

On the Define sheet of the Fortran block, Fortran variable XPROF of the type Block-Vec is defined using the Variable Definition dialog box.



Fortran variable	Definition
XPROF	Block-Vec Block=COLUMN Variable=X Sentence=COMPS



Variable name: ✓XPROF

Category
○ All
● Blocks
○ Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

Reference
Type: Block-Vec
Block: COLUMN
Variable: X
Sentence: COMPS

On the Fortran Fortran sheet, include these Fortran statements:

```
   WRITE(NTERM,10)
C* TOTAL NUMBER OF COMPONENTS IS 3 *
      NCOMP = 3
C* COMPONENT TO BE ACCESSED IS 2 *
      ICOMP = 2
C* STAGE TO BE ACCESSED IS 5 *
      ISTAGE = 5
C* CALCULATE INDEX INTO XPROF *
      II = NCOMP*(ISTAGE-1) + ICOMP
      WRITE(NTERM,20) XPROF(II)
   10 FORMAT(' * MOLE FRACTION OF 2ND COMPONENT ON 5TH STAGE
*')
   20 FORMAT(10X,F10.2)
```

Variables Dependent on Stage Number and Section Number

Examples of vector variables dependent on stage number and section number are the profile results of tray rating calculations. The values are stored as one-dimensional arrays. All stage values for section 1 are at the beginning, followed by all stage values for section 2, and so on. The number of components and the component order are the same as on the Components Specifications Selection sheet.

For a column with five stages and three sections, the flooding approach profile is stored as follows:

Array Index	Value for
1	Stage 1, section 1
2	Stage 2, section 1
3	Stage 3, section 1
4	Stage 4, section 1
5	Stage 5, section 1
6	Stage 1, section 2
.	
.	
.	
15	Stage 5, section 3

Variables Dependent on Stage Number and Operation Step Number

Examples of vector variables dependent on stage number and operation step number are temperature and flow profiles for BatchFrac. The values are stored as one-dimensional arrays. All stage values for operation step 1 are at the beginning, followed by all stage values for operation step 2, and so on.

For a BatchFrac block with four stages and three operation steps, the temperature profile is stored as follows:

Array Index	Value for
1	Stage 1, operation step 1
2	Stage 2, operation step 1
3	Stage 3, operation step 1
4	Stage 4, operation step 1
5	Stage 1, operation step 2
.	
.	
.	
12	Stage 4, operation step 3

Variables Dependent on Component Number, Stage Number, and Stripper Number

Examples of vector variables dependent on component number, stage number, and stripper number are the stripper composition profiles for PetroFrac. The values are stored as one-dimensional arrays. All component values for stage 1 of stripper 1 are at the beginning, followed by all component values for stage 2 of stripper 1, and so on. When Nstot is reached for stripper 1, the component and stage values for stripper 2 begin, and so on. Nstot denotes the total number of stages for that stripper.

For a PetroFrac block with three components, six stripper stages, and three strippers, the liquid composition profile is stored as follows:

Array Index	Value For
1	Component 1, stage 1, stripper 1
2	Component 2, stage 1, stripper 1
3	Component 3, stage 1, stripper 1
4	Component 1, stage 2, stripper 1
.	
.	
18	Component 3, Nstot, stripper 1
19	Component 1, stage 1, stripper 2
.	
.	
54	Component 3, Nstot, stripper 3

Variables Dependent on Component Number, Stage Number, and Operation Step Number

Examples of vector variables dependent on component number, stage number, and operation step number (opstep) are the composition profiles for BatchFrac. The values are stored as one-dimensional arrays. All component values for stage 1 of opstep 1 are at the beginning, followed by all component values for stage 2 of opstep 1, and so on. When Nstage is reached for opstep 1, the component and stage values for opstep 2 begin, and so on. Nstage denotes the number of stages in the column.

For a BatchFrac block with two components, three stages, and four opsteps, the liquid composition profile is stored as follows:

Array Index	Value for
1	Component 1, stage 1, opstep 1
2	Component 2, stage 1, opstep 1
3	Component 1, stage 2, opstep 1
.	

Continued

Array index	Value for
.	
6	Component 2, Nstage , opstep 1
7	Component 1, stage 1, opstep 2
.	
.	
24	Component 2, Nstage, opstep 3

Variables Dependent on Component Number, Accumulator Number, and Operation Step Number

The accumulator composition profile in BatchFrac is the only vector variable dependent on component number, accumulator number, and operation step number (opstep). The values are stored as a one-dimensional array. All component values for accumulator 1 of opstep 1 are at the beginning, followed by all the component values for accumulator 2 of opstep 1, and so on. Naccum denotes the total number of accumulators in the column. When Naccum is reached for opstep 1, the component and accumulator values for opstep 2 begin, and so on.

For a BatchFrac block with two components, three accumulators, and four opsteps, the accumulator composition profile is stored as follows:

Array Index	Value for
1	Component 1, accumulator 1, opstep 1
2	Component 2, accumulator 1, opstep 1
3	Component 1, accumulator 2, opstep 1
.	
.	
6	Component 2, Naccum, opstep 1
7	Component 1, accumulator 1, opstep 2
.	
.	
24	Component 2, Naccum, opstep 4

MHeatX Profiles

You can use the Block-Vec variable type to access the temperature difference between the hot side and cold side of an MHeatX block:

Variable	Description
DT	Temperature approach profile, including points added for phase change points and points for streams entering and leaving the exchanger.
DTBASE	Temperature approach profile for base points only. The length of the vector is the Number of Zones + 1. The Number of Zones is specified on the MHeatX Input ZoneAnalysis sheet.

Reactor Profiles

You can use the Block-Vec variable type to access RBatch time profiles and RPlug length profiles for variables such as calculated temperature and pressure. Values are stored at each output point. The length of the vector is the number of output points +1.

For example, the temperature profile for an RBatch reactor that runs for 10 hours with output points each hour would be stored as follows:

Array Index	Temperature at
1	Initial conditions
2	1 hour
3	2 hours
.	
.	
.	
11	10 hours

The output intervals are determined as follows:

Model	Output Interval
Rplug	Number of Profile Points along the reactor length, specified on the RPlug Report Profiles sheet
Rbatch	Time Interval Between Profile Points, specified on the RBatch Setup Operation Times sheet.

Accessing Property Parameter Vectors

You can access the vector of coefficients of temperature-dependent property parameters.

Variable type	Description
Un-Cor-Vec	Temperature-dependent pure component property parameter vector
Bi-Cor-Vec	Temperature-dependent binary property parameter vector

Aspen Plus automatically:

- Interprets the Fortran variable you assign to the profile as an array variable
- Dimensions the variable

Aspen Plus generates a variable by adding the letter L to the beginning of the Fortran variable name you assigned to the vector. The value of this variable is the length of the vector.

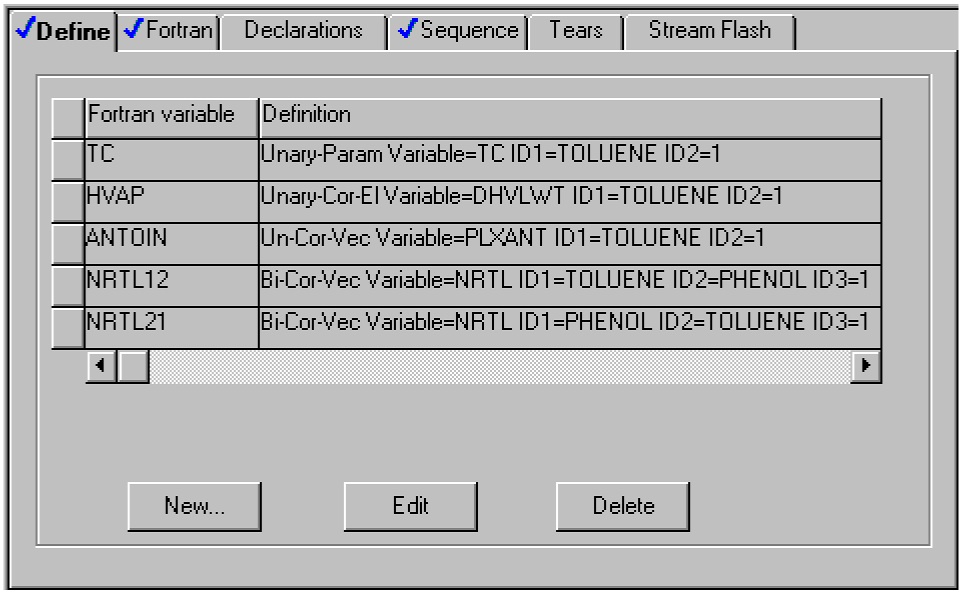
Accessed property parameter vectors are always in SI units.

See *Aspen Plus Physical Property Methods and Models*, Chapter 3, for the length and contents of each temperature-dependent property parameter. You can also obtain this information by using Help from the Properties Parameters PureComponent and Properties Parameters Binary sheets.

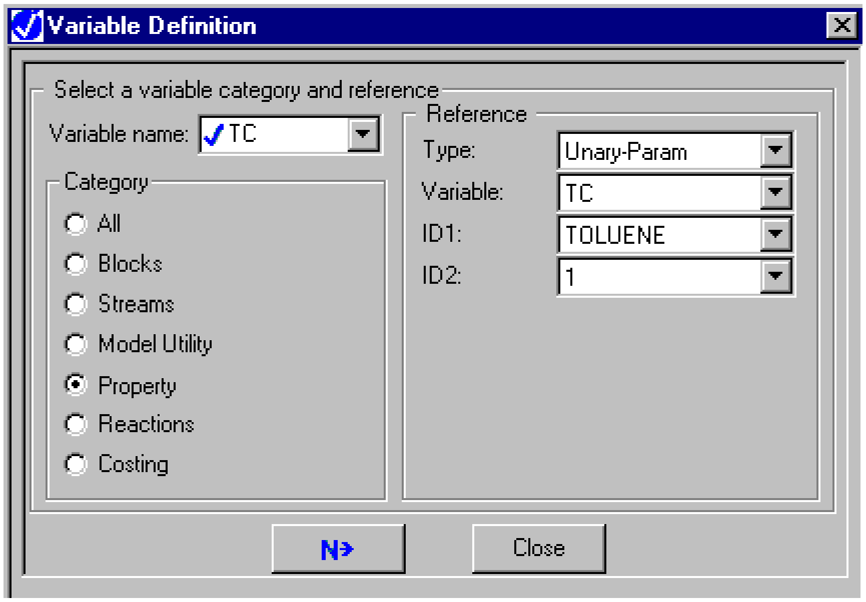
Example for Accessing Property Parameters

On the following Define sheet all references are to dataset 1.

This variable	Accesses the
TC	Critical temperature of component TOLUENE
HVAP	Heat of vaporization of component TOLUENE. Heat of vaporization is the first element of the temperature-dependent Watson parameter DHVLWT.
ANTOIN	Antoine vapor pressure coefficients parameter PLXANT as a vector.
REN12	NRTL parameter vector for the TOLUENE-PHENOL binary
REN21	NRTL parameter vector for the PHENOL-TOLUENE binary



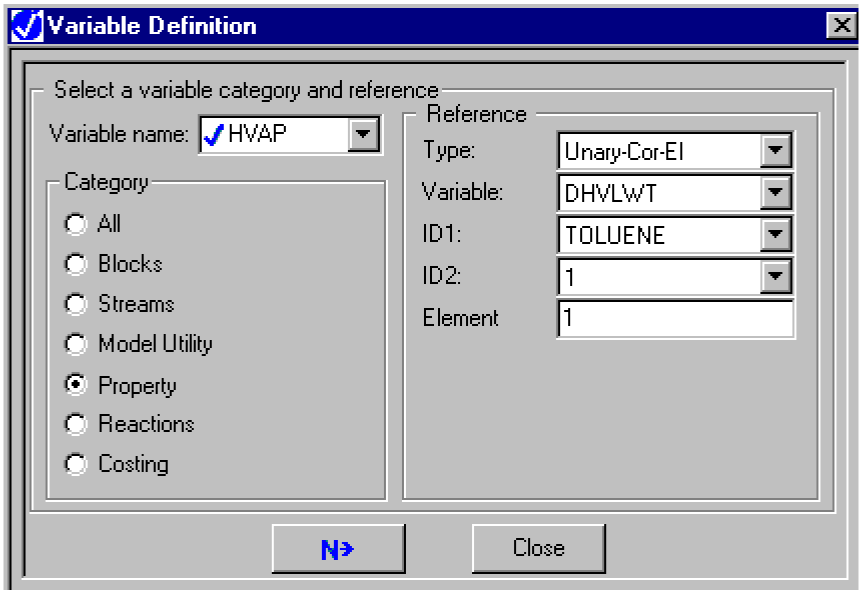
Fortran variable	Definition
TC	Unary-Param Variable=TC ID1=TOLUENE ID2=1
HVAP	Unary-Cor-El Variable=DHVLWT ID1=TOLUENE ID2=1
ANTOIN	Un-Cor-Vec Variable=PLXANT ID1=TOLUENE ID2=1
NRTL12	Bi-Cor-Vec Variable=NRTL ID1=TOLUENE ID2=PHENOL ID3=1
NRTL21	Bi-Cor-Vec Variable=NRTL ID1=PHENOL ID2=TOLUENE ID3=1



Variable name: ✓TC

Category
○ All
○ Blocks
○ Streams
○ Model Utility
● Property
○ Reactions
○ Costing

Reference
Type: Unary-Param
Variable: TC
ID1: TOLUENE
ID2: 1



Variable name: HVAP

● Property

Reference

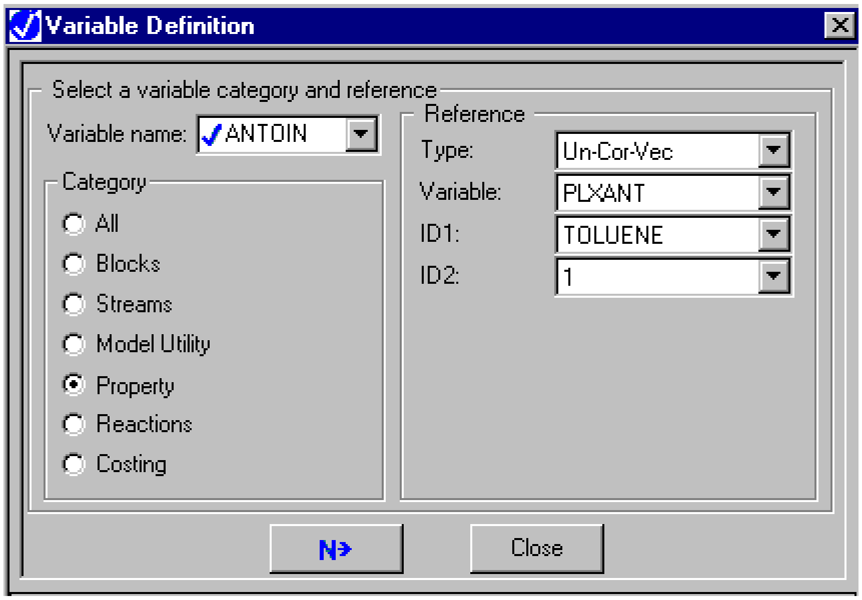
Type: Unary-Cor-El

Variable: DHVLWT

ID1: TOLUENE

ID2: 1

Element 1



Variable name: ANTOIN

● Property

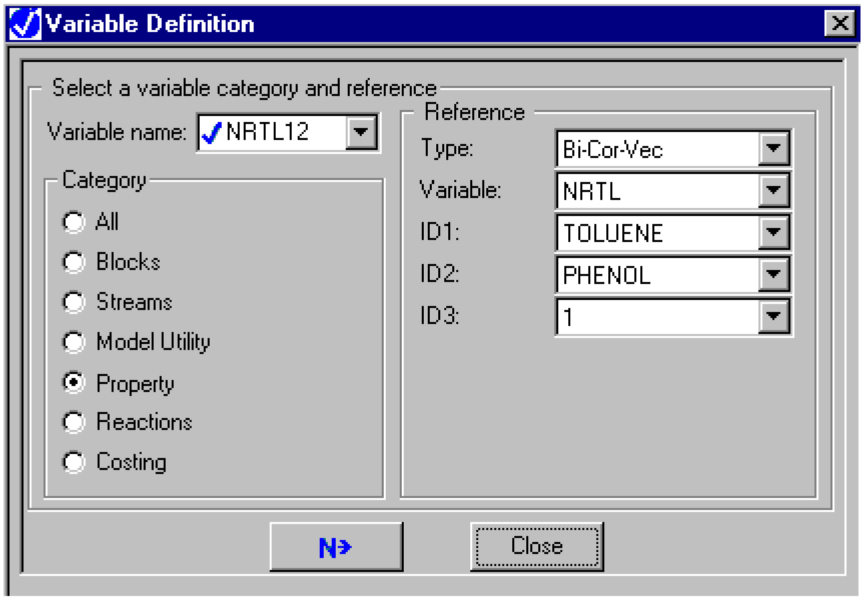
Reference

Type: Un-Cor-Vec

Variable: PLXANT

ID1: TOLUENE

ID2: 1



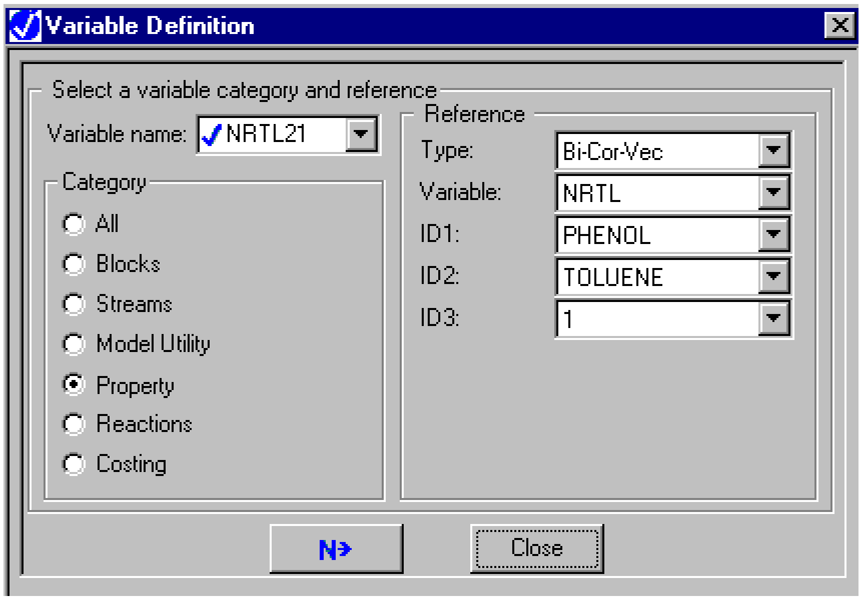
Variable Definition

Select a variable category and reference

Variable name: NRTL12

Category
- ○ All
- ○ Blocks
- ○ Streams
- ○ Model Utility
- ● Property
- ○ Reactions
- ○ Costing

Reference
Type: Bi-Cor-Vec
Variable: NRTL
ID1: TOLUENE
ID2: PHENOL
ID3: 1



Variable Definition

Select a variable category and reference

Variable name: NRTL21

Category
- ○ All
- ○ Blocks
- ○ Streams
- ○ Model Utility
- ● Property
- ○ Reactions
- ○ Costing

Reference
Type: Bi-Cor-Vec
Variable: NRTL
ID1: PHENOL
ID2: TOLUENE
ID3: 1

◆ ◆ ◆ ◆

19 Fortran Blocks and In-Line Fortran

Aspen Plus lets you insert your own Fortran statements into flowsheet computations. This chapter describes:

- Using Fortran in Aspen Plus
- Fortran Blocks
- Creating a Fortran block
- Entering Fortran statements
- Specifying when to execute a Fortran block
- Rules for writing Fortran statements

Using Fortran in Aspen Plus

You can use Fortran in Aspen Plus to perform any task that can be written as valid Fortran expressions.

You can input Fortran expressions in a number of ways in Aspen Plus:

- In Fortran blocks
- On the Fortran sheets of other blocks, such as design specifications, sensitivity or optimization problems
- In external Fortran subroutines

Fortran blocks:

- Contain Fortran expressions used to perform user-defined tasks
- Can read and/or write flowsheet variables
- Are executed at a specific point in the simulation

Aspen Plus checks your Fortran code interactively as you enter it so most syntax errors are detected before a run. If the status indicator on a Fortran sheet is ◒, use Next to find out what is incomplete.

You can write external User Fortran subroutines when the models provided by Aspen Plus do not meet your needs. After you compile these subroutines, they are dynamically linked when the simulation is run. Aspen Plus allows extensive customization of the models through the use of these external user subroutines. For more information on external user subroutines, see *Aspen Plus User Models*.

Aspen Plus can interpret most in-line Fortran. Fortran that cannot be interpreted is compiled and dynamically linked to the Aspen Plus module. Because dynamic linking is used, the overhead for in-line Fortran requiring compilation is small.

Note If the Fortran cannot be interpreted, a FORTRAN compiler is needed. For the recommended compiler for a given platform, see the relevant Aspen Plus installation guide.

About Fortran Blocks

Fortran blocks let you insert Fortran statements into flowsheet computations to perform user-defined tasks, such as:

- Calculating and setting input variables before they are used (feedforward control)
- Writing information to the Control Panel
- Reading input from a file
- Writing results to the Aspen Plus report or to any external file
- Calling external subroutines
- Writing your own user models

Since Aspen Plus is a sequential modular simulator that executes one unit operation at a time, you must specify where in the sequence of unit operations each Fortran block is to be executed. You can do this by specifying one of these:

- Which flowsheet variables are read from and written to in the Fortran block
- The position of the Fortran block in the list of unit operation blocks

This lets Aspen Plus determine when the Fortran block should be executed. It is recommended that you allow Aspen Plus to determine the execution sequence of a Fortran block.

Define a Fortran block by:

1. Creating the Fortran block.
2. Identifying the flowsheet variables that the block samples or manipulates.
3. Entering the Fortran statements.
4. Specifying when the Fortran block is executed.

Creating a Fortran Block

To create a Fortran block:

1. From the Data menu, point to Flowsheeting Options, then Fortran.
2. In the Fortran Object Manager, click New.
3. In the Create New ID dialog box, enter an ID or accept the default, and click OK.

The following sections describe how to complete the required sheets.

Identifying Flowsheet Variables

You must identify the flowsheet variables used in a Fortran block and assign them variable names. A variable name identifies a flowsheet variable on other Fortran block sheets.

Using the Define Sheet to Identify Flowsheet Variables

Use the Define sheet to identify a flowsheet variable and assign it a variable name. When completing a Define sheet, specify the variables on the Variable Definition dialog box. The Define sheet shows a concise summary of all the accessed variables, but you cannot modify the variables on the Define sheet.

On the Define sheet:

1. To create a new variable, click the New button.

   – or –

   To edit an existing variable, select a variable and click the Edit button.
2. Type the name of the variable in the Variable Name field.

   A variable name must:

   - Be six characters or less for a scalar variable
   - Be five characters or less for a vector variable
   - Start with an alphabetic character (A – Z)
   - Have subsequent alphanumeric characters (A – Z, 0 – 9)
   - Not begin with IZ or ZZ
3. In the Category frame, use the option button to select the variable category.
4. In the Reference frame, select the variable type from the list in the Type field.

   Aspen Plus displays the other fields necessary to complete the variable definition.
5. Click Close to return to the Define sheet.

For more information on accessing variables, see Chapter 18.

Tips Use the Delete button to quickly delete a variable and all of the fields used to define it. Use the Edit button to modify the definition of a variable in the Variable Definition dialog box.

Entering Fortran Statements and Declarations

You can enter Fortran statements:

- On the Fortran sheet
- In your text editor (for example, Notepad), and then copy and paste them onto the Fortran sheet

Enter Fortran declarations in the same way as executable Fortran statements, using the Declarations sheet instead of the Fortran sheet.

You can include any Fortran declarations in a Fortran block, such as:

- Include statements
- COMMON definitions
- DIMENSION definitions
- Data type definitions (INTEGER and REAL)

If a Fortran variable meets one of these criteria, you should place it in a COMMON:

- It is also used by another block.
- Its value must be retained from one iteration of a Fortran block to another.

Fortran variables that you defined on the Define sheet should not be declared on the Declarations sheet.

Using the Fortran Sheet

To enter executable Fortran statements on the Fortran sheet:

1. Click the Fortran tab on the Fortran form.

   To review rules and restrictions for in-line Fortran, see Rules for In-Line Fortran Statements, this chapter.

2. Enter your Fortran statements.
3. To ensure that you enter accurate variable names, click the right mouse button. In the popup menu, click Variable List.

   The Defined Variable List window appears. You can drag and drop the variables from the Defined Variable List to the Fortran sheet.

Specifying When Fortran Statements Are Executed

You must specify when a Fortran block will be executed during calculations. To do this:

1. On the Fortran form, click the Sequence sheet.
2. In the Read Variables field, specify which variables are used but not changed. In the Write Variables field, specify which variables are changed.

   – or –

   In the Execute field on the Sequence sheet, specify when to execute the block.

Option	When Executed
First	At the beginning of a simulation
Before	Before a block. Specify the block type and name.
After	After a block. Specify the block type and name.
Last	At the end of a simulation
Report	While the report is being generated
Based on order in sequence	As specified on the Convergence Sequence Specification sheet
Use Read/Write Variables	Aspen Plus uses read and write variables to automatically sequence the Fortran block.

Read Variables and Write Variables are used to establish which of the variables appearing on the Define sheet are only sampled variables, and which are changed by the Fortran block.

Read Variables establish information flow from the block or stream containing a sampled (read-only) variable to the Fortran block.

Write Variables establish information flow from the Fortran block to changed (read-write or write-only) variables.

If the automatic sequencing logic using Read Variables and Write Variables does not appear to work properly, use the Execute statement to specify explicitly when the block is executed.

Converging Loops Introduced by Fortran Blocks

A Fortran block can introduce loops that must be solved iteratively.

For example, a Fortran block can change an upstream variable based on the value of a downstream variable. This could occur if the Fortran block was being used to set a makeup stream based on the product flowrates.

If you are using Fortran blocks that create loops, you must specify Read Variables and Write Variables for Aspen Plus to detect the loops and produce correct simulation results.

Aspen Plus automatically solves any loops introduced by the Fortran block, if you:

- Check the Tear Fortran Write Variables on the Convergence Conv-Options Defaults Sequencing sheet
- Specify Read Variables and Write Variables on the Fortran block Sequence sheet.

When a Fortran block creates a loop, variables entered as Write Variables can be torn for convergence in the same way as recycle streams. Aspen Plus can do this automatically, or you can specify tear variables.

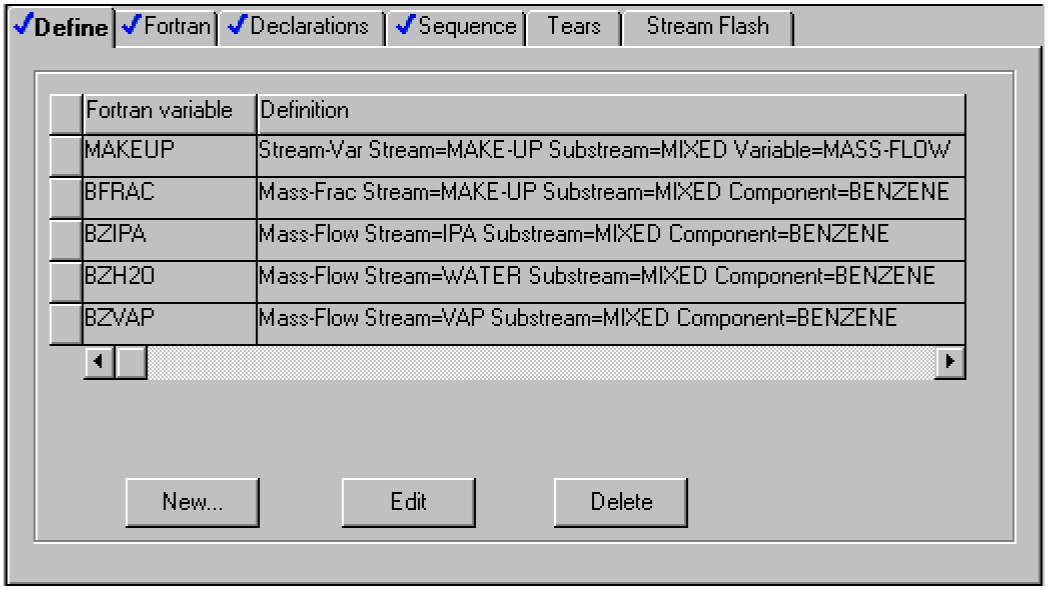
To specify a Fortran Write Variable as a tear variable:

1. On the Fortran form, click the Tears tab.
2. In the Tear Variable Name field, select a variable you entered in the Write Variable field on the Sequence sheet.
3. Enter lower and upper bounds for the tear variable in the Lower Bound and Upper Bound fields.

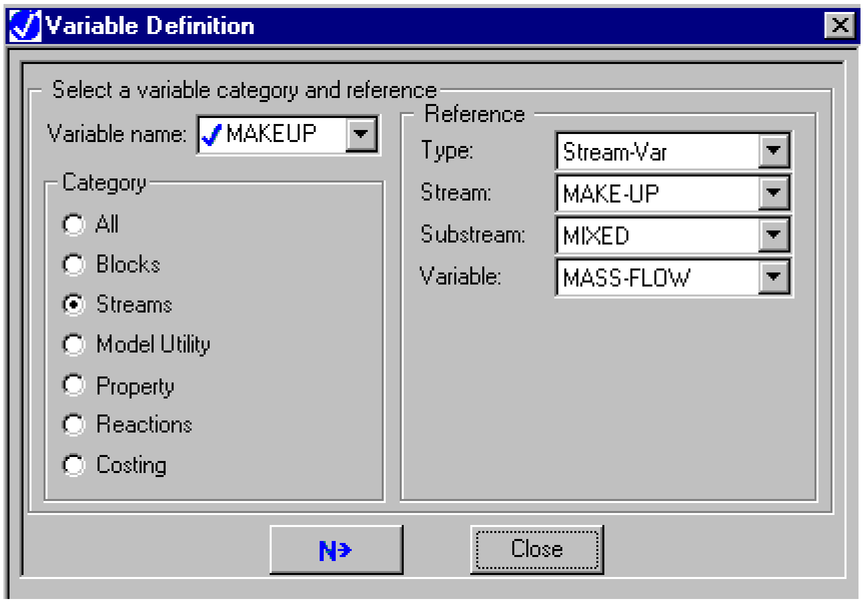
The tear variable will be solved along with recycle tears to converge the flowsheet. See Chapter 17, Convergence, for more information on flowsheet convergence.

Example of Calculating Make-Up Flow Rate

The mass flow rate of make-up stream MAKEUP is determined by the amount of benzene in the outlet streams from the flowsheet. The variables are selected using the Variable Definition dialog box. In order for the simulation to converge correctly, the Tear Fortran Write Variables needs to be selected on the Convergence Conv-Options Defaults Sequencing sheet.



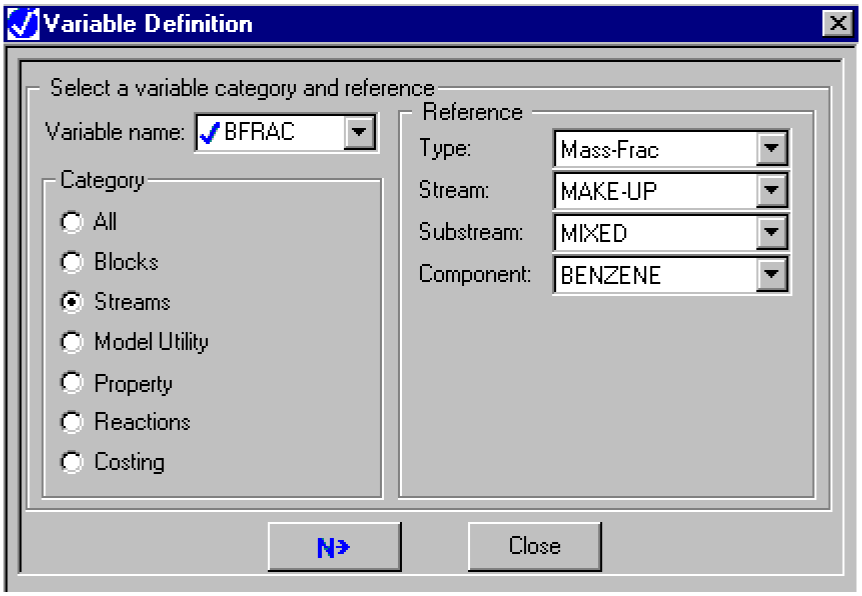
Fortran variable	Definition
MAKEUP	Stream-Var Stream=MAKE-UP Substream=MIXED Variable=MASS-FLOW
BFRAC	Mass-Frac Stream=MAKE-UP Substream=MIXED Component=BENZENE
BZIPA	Mass-Flow Stream=IPA Substream=MIXED Component=BENZENE
BZH2O	Mass-Flow Stream=WATER Substream=MIXED Component=BENZENE
BZVAP	Mass-Flow Stream=VAP Substream=MIXED Component=BENZENE



Variable name: ✓ MAKEUP

Category
- ○ All
- ○ Blocks
- ● Streams
- ○ Model Utility
- ○ Property
- ○ Reactions
- ○ Costing

Reference
Type: Stream-Var
Stream: MAKE-UP
Substream: MIXED
Variable: MASS-FLOW



Variable Definition

Select a variable category and reference

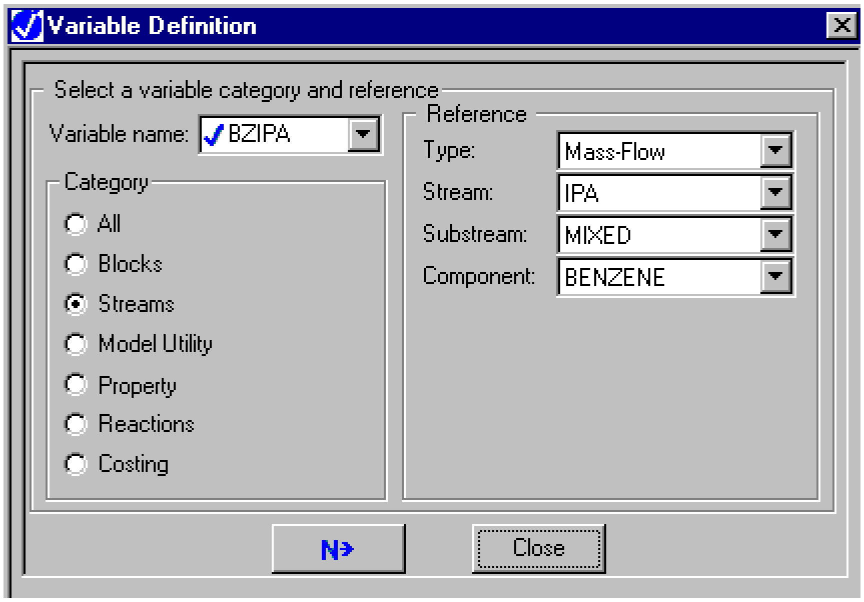
Variable name: BFRAC

Category

○ All
○ Blocks
● Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

Reference

Type: Mass-Frac
Stream: MAKE-UP
Substream: MIXED
Component: BENZENE



Variable Definition

Select a variable category and reference

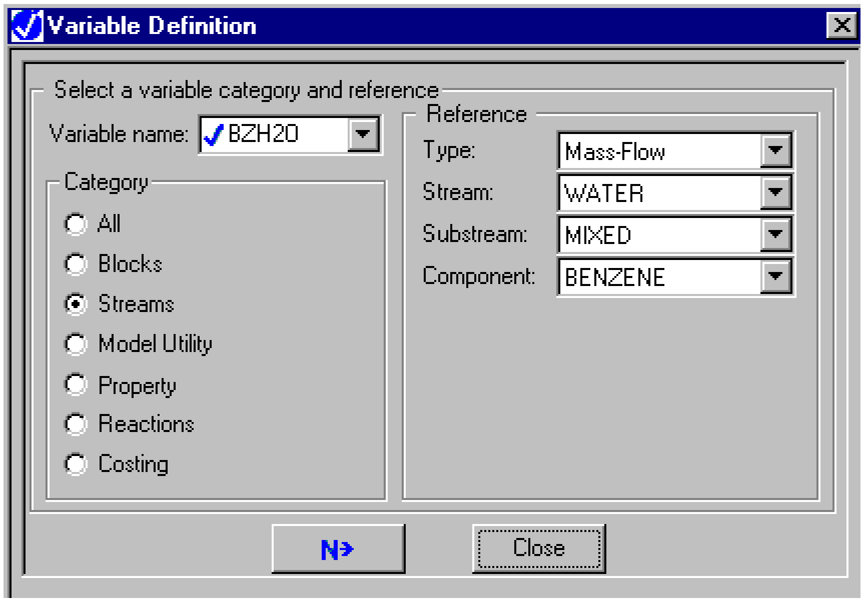
Variable name: BZIPA

Category

○ All
○ Blocks
● Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

Reference

Type: Mass-Flow
Stream: IPA
Substream: MIXED
Component: BENZENE



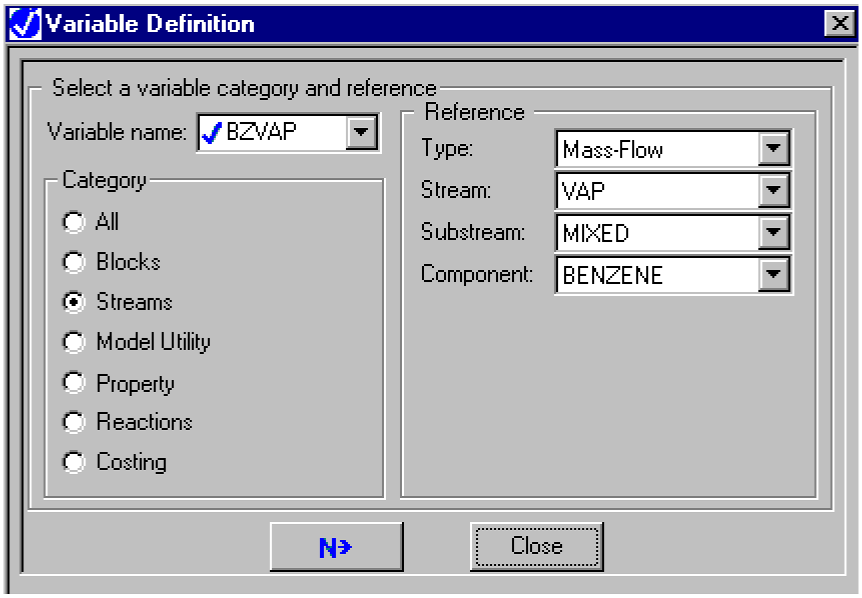
Variable Definition

Select a variable category and reference

Variable name: BZH2O

Category
○ All
○ Blocks
● Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

Reference
Type: Mass-Flow
Stream: WATER
Substream: MIXED
Component: BENZENE



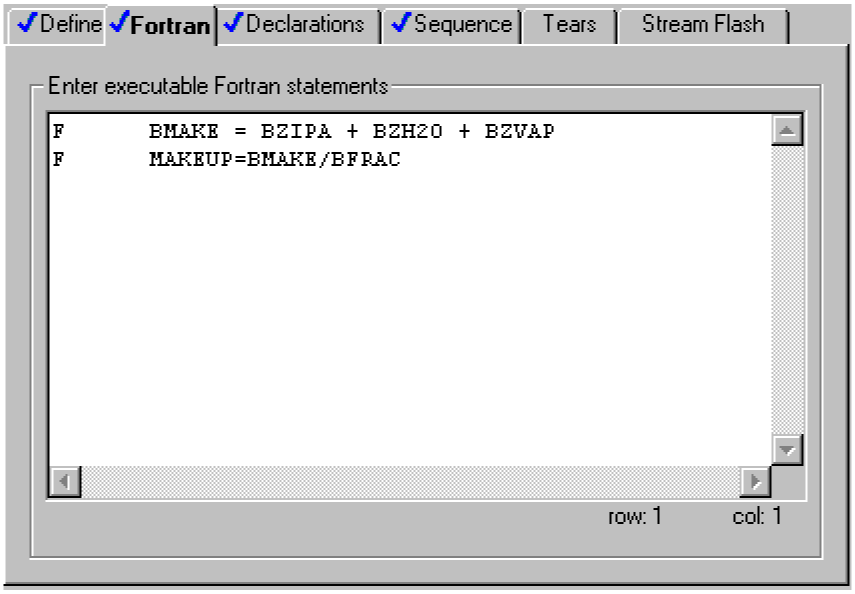
Variable Definition

Select a variable category and reference

Variable name: BZVAP

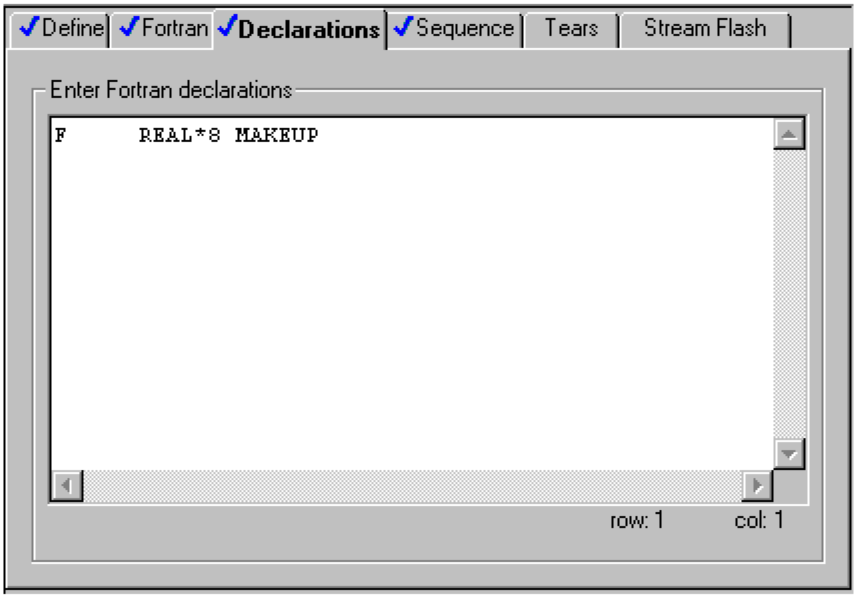
Category
○ All
○ Blocks
● Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

Reference
Type: Mass-Flow
Stream: VAP
Substream: MIXED
Component: BENZENE



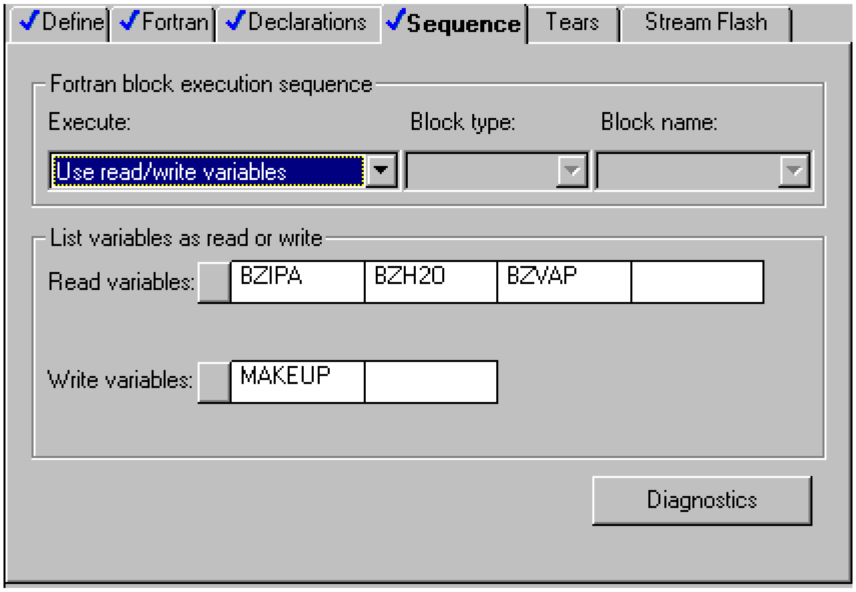
Enter executable Fortran statements

```
F       BMAKE = BZIPA + BZH2O + BZVAP
F       MAKEUP=BMAKE/BFRAC
```



Enter Fortran declarations

```
F      REAL*8 MAKEUP
```



Fortran block execution sequence

Execute: Use read/write variables

Block type:

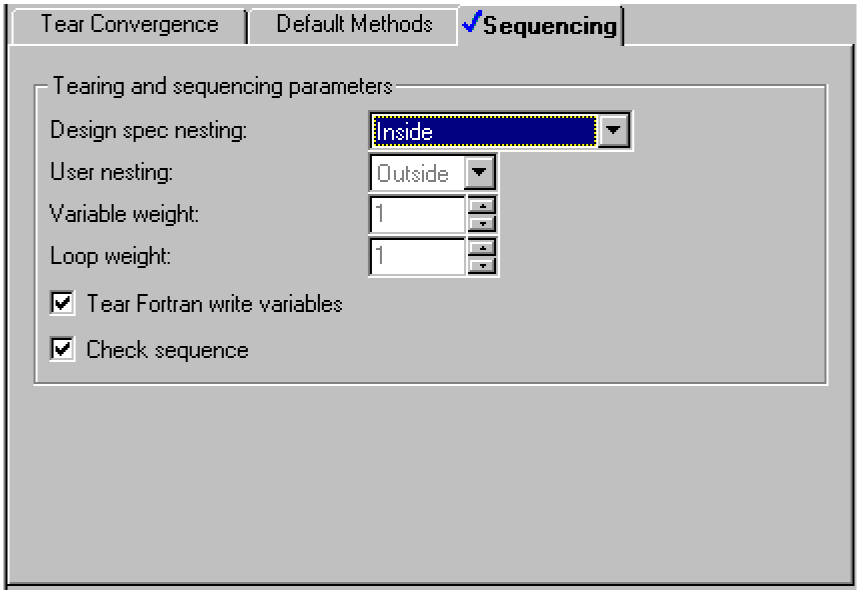
Block name:

List variables as read or write

Read variables: BZIPA BZH20 BZVAP

Write variables: MAKEUP

On the Convergence Conv-Options Defaults Sequencing sheet, Tear Fortran Write Variables is selected:



Tearing and sequencing parameters

Design spec nesting: Inside

User nesting: Outside

Variable weight: 1

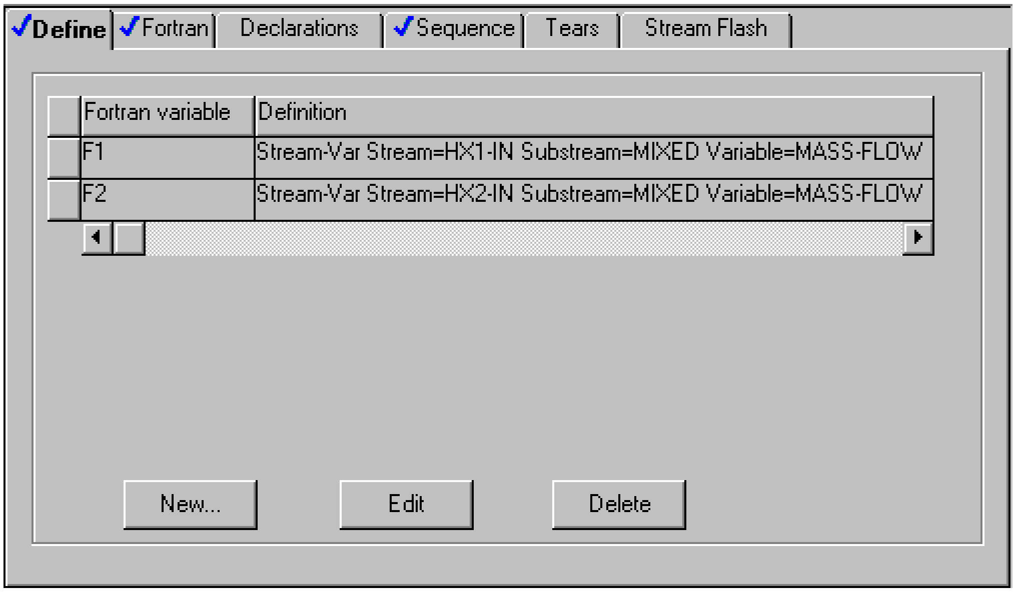
Loop weight: 1

☑ Tear Fortran write variables

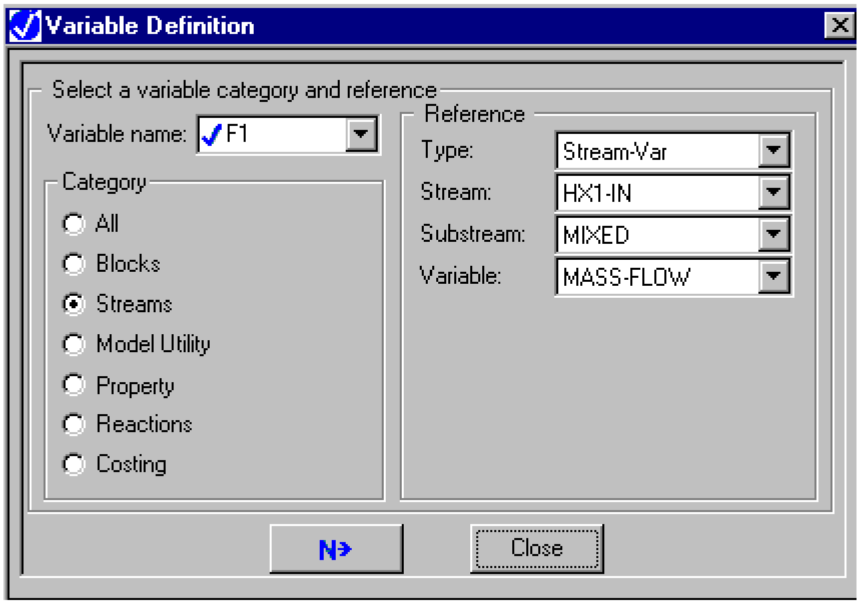
☑ Check sequence

Example of Feedforward Control of Stream Feedrate

A Fortran block is used to set the feedrate of stream HX2 to equal 75% of the stream HX1.



Fortran variable	Definition
F1	Stream-Var Stream=HX1-IN Substream=MIXED Variable=MASS-FLOW
F2	Stream-Var Stream=HX2-IN Substream=MIXED Variable=MASS-FLOW



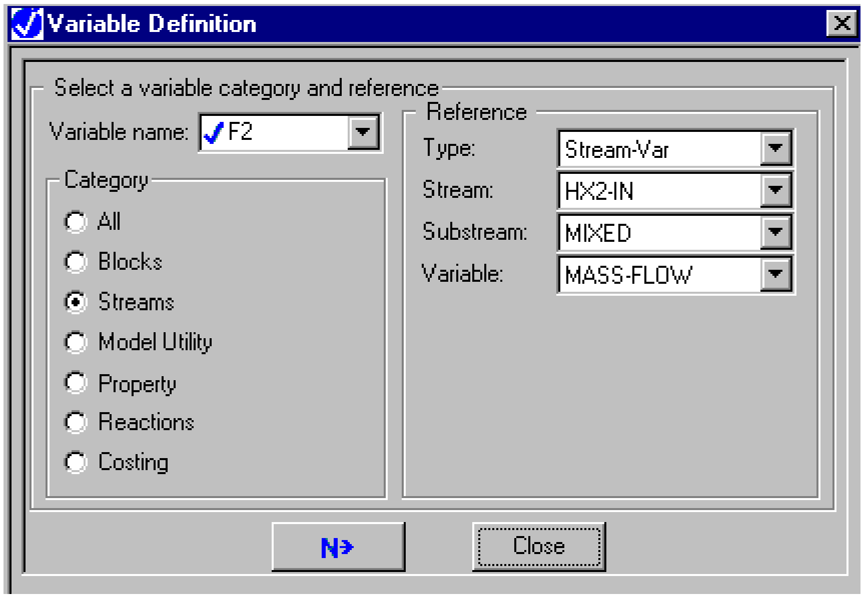
Variable name: ✓F1

Type: Stream-Var

Stream: HX1-IN

Substream: MIXED

Variable: MASS-FLOW



Variable name: F2

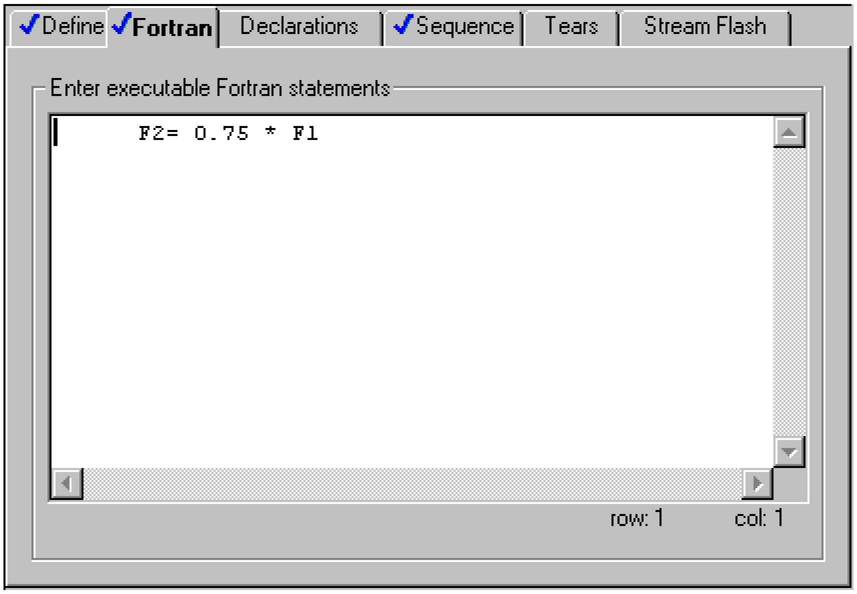
Category: ○ All ○ Blocks ● Streams ○ Model Utility ○ Property ○ Reactions ○ Costing

Type: Stream-Var

Stream: HX2-IN

Substream: MIXED

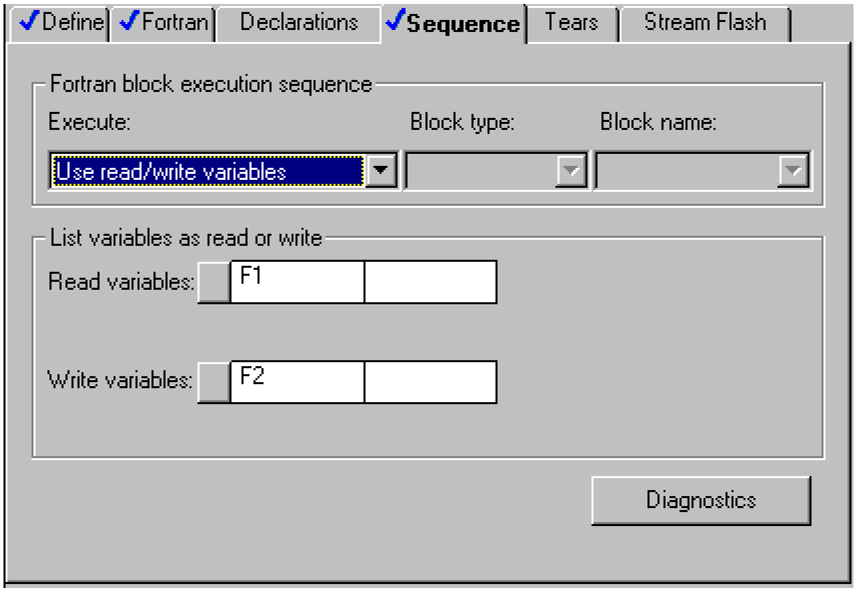
Variable: MASS-FLOW



Enter executable Fortran statements

```
      F2= 0.75 * F1
```

row: 1 col: 1



Fortran block execution sequence

Execute: Use read/write variables

Block type:

Block name:

List variables as read or write

Read variables: F1

Write variables: F2

Rules for In-Line Fortran Statements

To achieve successful compilation of your Fortran statements, follow these rules:

- By default, variables beginning with A through H, or O through Z, are double precision real. Variables beginning with I through N are integer. Use double precision functions (for example, DSQRT) and double precision constants (for example, 1D0).

- Do not use variable names beginning with IZ or ZZ.
- Because Fortran is column-sensitive, this table shows how to do certain things:

To do this	Use
Indicate comments	Column one for C and leave column two blank
Enter statement labels	Only columns three, four, and five
Begin executable statements	Column seven or beyond

- You can call your own subroutines or functions. You can use labeled or blank (unlabeled) COMMON blocks.
- Fortran variables you define on the Specification sheet cannot be placed in a COMMON.
- Do not use IMPLICIT, SUBROUTINE, ENTRY, RETURN, END statements, nor arithmetic statement functions.

Disabling Syntax Checking

By default, Aspen Plus interactively checks your Fortran statements. You can turn off interactive syntax checking. You might need to do this, for example, if you are using a compiler that accepts nonstandard Fortran extensions, or if the syntax checker incorrectly flags correct Fortran as incomplete.

To turn off Fortran syntax checking:

1. From the Tools menu, click Options.
2. Ensure the Check Inline Fortran for Syntax Errors checkbox is clear.

Writing to the Screen and Aspen Plus Files

In Fortran WRITE statements, you can use the following predefined variables for the unit number:

Unit	Destination
NTERM	Control Panel (if running from the user interface) Terminal (if running interactively outside of the user interface), or Log file (if running batch)
NRPT	Aspen Plus report
NHSTRY	Simulation history

Examples:

For writing to the Control Panel, enter:

```
WRITE(NTERM, *) A,B, C, X
```

For writing to the report file, enter:

```
WRITE(NRPT, *) A, B, C, X
```

If writing to the Aspen Plus report from a Fortran block, select Report in the Execute field on the Sequence Sheet. Output written to the report file will appear in the Flowsheet section of the Fortran block report.

When writing to a user-defined file, use a Fortran unit number between 50 and 100.

Interactive Read Statements

In Fortran READ statements you can use the predefined variable NTERM for the unit number for interactive input.

This table shows what the predefined variable does:

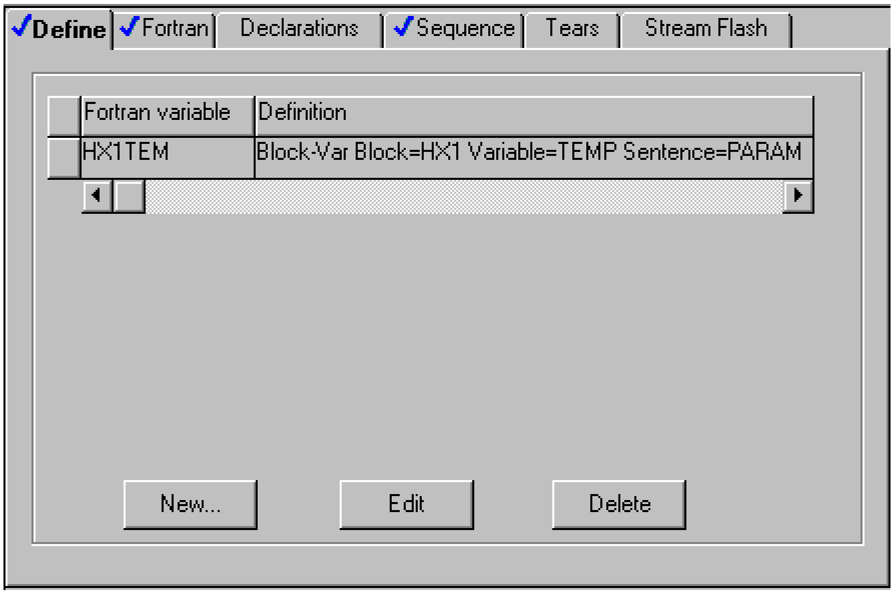
If you are running interactively	Then READ (NTERM [†])
From the user interface	Displays a dialog box accepting up to one line of input
Outside the user interface	Pauses for input from the terminal

[†] ***Do not read from NTERM when running batch.***

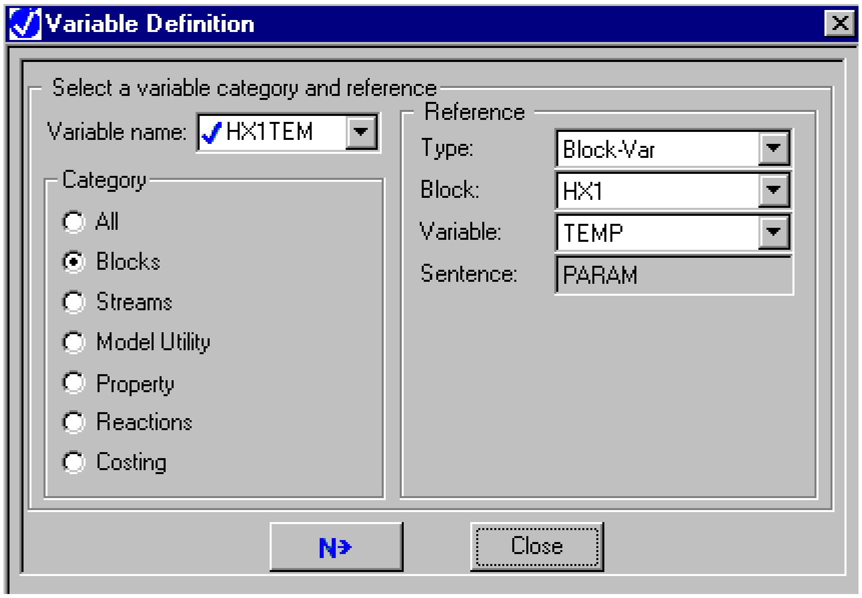
Example of Interactive READ from a Fortran block

A Fortran block pauses for user input of the temperature for block HX1 before executing the block.

The following form defines the variable HX1TEM as the temperature input specification for block HX1:



Fortran variable	Definition
HX1TEM	Block-Var Block=HX1 Variable=TEMP Sentence=PARAM

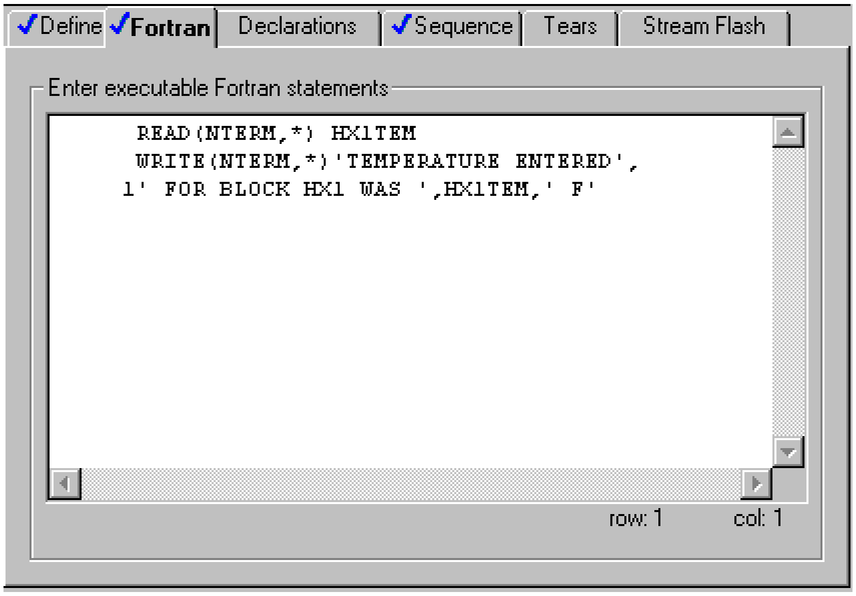


Variable name: HX1TEM

○ All
● Blocks
○ Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

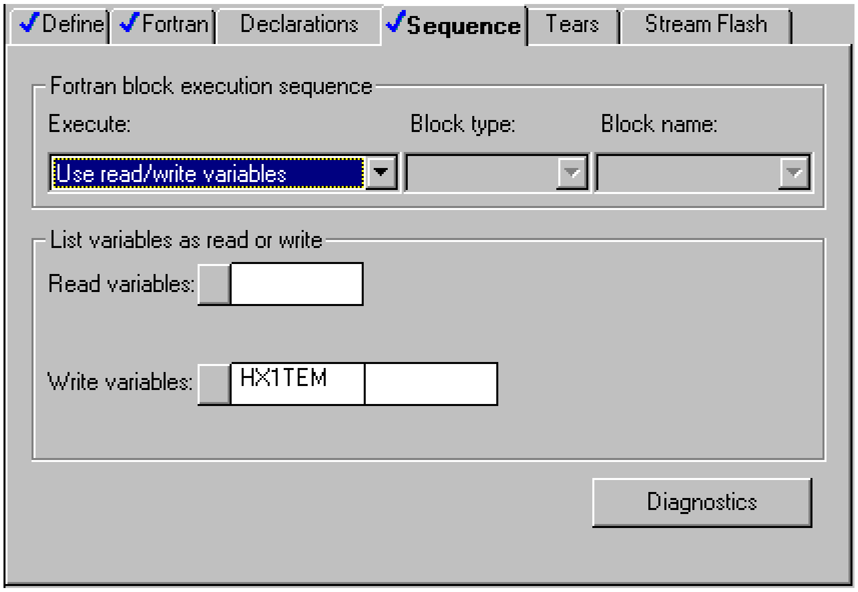
Type: Block-Var
Block: HX1
Variable: TEMP
Sentence: PARAM

The Fortran statements read HX1TEM from interactive screen input, and echo the value to the control panel:



```
      READ(NTERM,*) HX1TEM
      WRITE(NTERM,*)'TEMPERATURE ENTERED',
     1' FOR BLOCK HX1 WAS ',HX1TEM,' F'
```

The Sequence sheet specifies that HX1TEM is a write variable, so that Aspen Plus can sequence the Fortran block.



Execute: Use read/write variables

Block type:

Block name:

List variables as read or write

Read variables:

Write variables: HX1TEM

Retaining Variables Between Iterations and Blocks

Place a Fortran variable in a COMMON (on the Declarations sheet) if you want to do one of the following:

- Retain the value of the variable from one calculation pass to another
- Use the same variable in more than one block

The COMMON statement must appear in each block where the variable is used.

About the Interpreter

By default, Aspen Plus will interpret in-line Fortran if it is possible. Fortran that cannot be interpreted is compiled and linked into a shared library or dynamic link library (DLL). A Fortran compiler is needed for compiling the code. (See the appropriate installation guide for the recommended compiler for a given platform.) It is possible to compile all of the Fortran, by selecting Write Inline Fortran to a Subroutine to be Compiled and Dynamically Linked on the Setup SimulationOptions System sheet.

The following Fortran can be interpreted:

- Arithmetic expressions and assignment statements
- IF statements
- GOTO statements, except assigned GOTO
- WRITE statements that use the built-in unit number variables NTERM, NRPT, or NHSTRY
- FORMAT statements
- CONTINUE statements
- DO loops
- Calls to these built-in Fortran functions:

DABS
DACOS
DASIN
DATAN
DATAN2
DCOS
DCOSH
DCOTAN
DERF
DEXP
DFLOAT
DGAMMA
DLGAMA
DLOG
DLOG10
DMAX1
DMIN1
DMOD
DSIN
DSINH
DSQRT
DTAN
DTANH
IABS
IDINT
MAX0
MIN0
MOD

You can also use the equivalent single precision or generic function names. But, Aspen Plus always performs double precision calculations.

If you use the following statements, you must enter them on the Declaration sheet:

- REAL or INTEGER statements
- DOUBLE PRECISION statements
- DIMENSION statements
- COMMON statements

The following statements require compilation:

CALL	LOGICAL
CHARACTER	PARAMETER
COMPLEX	PRINT
DATA	RETURN
ENTRY	READ
EQUIVALENCE	STOP
IMPLICIT	SUBROUTINE

About External Fortran Subroutines

External user Fortran is an open and extensive customization capability in Aspen Plus. An Aspen Plus user model consists of one or more Fortran subroutines that you write yourself when the models provided by Aspen Plus do not meet your needs. A proper argument list is needed in the subroutine to interface your user model to Aspen Plus.

You can write six kinds of user models for use in Aspen Plus:

External Fortran Application Types	Use
User Unit Operation Models	Units not represented by Aspen Plus unit operation models
Kinetic Models	Reactors, Reactive Distillation, Pressure Relief
Physical Property Models	Pure and mixture, activity models, KLL, user equations-of-state
Stream Properties	Special properties to be calculated for a stream
Unit Operation Customization	Reactor heat transfer, column hydraulics, LMTD correction, pressure drop, liquid-liquid distribution coefficients
Customized Reports	User-defined stream report, user block reports, applications based on the Summary File Toolkit
Sizing and Costing	User cost blocks

Templates that include the argument list and other useful code for starting a user model are provided in the Templates directories where Aspen Plus is installed. For more information on how to write a user model, see *Aspen Plus User Models*.

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20 Sensitivity

This chapter explains how to use sensitivity analysis to examine the sensitivity of a process to key variables including:

- What is sensitivity analysis?
- Defining a sensitivity block
- Specifying sampled and manipulated variables
- Defining tabulated variables
- Optional Fortran statements
- Examples

About Sensitivity Analysis

Sensitivity analysis is a tool for determining how a process reacts to varying key operating and design variables. You can use it to vary one or more flowsheet variables and study the effect of that variation on other flowsheet variables. It is a valuable tool for performing “what if” studies. The flowsheet variables that are varied must be inputs to the flowsheet. They can not be variables that are calculated during the simulation.

You can use sensitivity analysis to verify if the solution to a design specification lies within the range of the manipulated variable. You can also use it to perform simple process optimization.

You can use sensitivity blocks to generate tables and/or plots of simulation results as functions of feed stream, block input, or other input variables. Sensitivity analysis results are reported in a table on the Sensitivity Results Summary sheet. The first *n* columns of the table list the values of the variables that are varied, where *n* is the number of varied flowsheet variables entered on the Sensitivity Input Vary sheet. The remaining columns in the table contain the values of variables that you tabulated on the Tabulate sheet. The tabulated results can be any flowsheet variable or any valid Fortran expression that may depend on flowsheet variables that are either input or calculated.

The results can be plotted using the Plot Wizard from the Plot menu to easily visualize the relationships between different variables. See Chapter 13 for more information about the Plot Wizard.

Sensitivity blocks provide additional information to base-case results, but have no effect on the base-case simulation. The simulation runs independently of the sensitivity study.

Sensitivity blocks with more than one varied variable generate a row in the sensitivity table for each combination of values. If you are interested in the sensitivity to more than one variable with each varied independently, use a separate sensitivity block for each varied variable.

Sensitivity blocks create loops that must be evaluated once for each row of the sensitivity table. Aspen Plus sequences sensitivity blocks automatically. Or, you can sequence a sensitivity block using the Convergence Sequence Specifications sheet.

Accessed scalar flowsheet variables are in the units set selected for the sensitivity block. You cannot modify the units individually for different variables in the sensitivity. You can either change the unit set for the sensitivity block (on the toolbar of the Data Browser), or enter an expression on the tabulate sheet to convert the variable. Accessed vector variables are always in SI units.

Defining a Sensitivity Block

Define a sensitivity block by:

1. Creating the sensitivity block
2. Identifying the sampled flowsheet variables
3. Identifying the input variables to manipulate to generate the table
4. Defining what you want Aspen Plus to tabulate
5. Entering optional Fortran statements

Creating a Sensitivity Block

To create a sensitivity block:

1. From the Data menu, click Model Analysis Tools, then Sensitivity.
2. On the Sensitivity Object Manager, click Create.
3. In the Create New ID dialog box, enter an ID or accept the default, and click OK. In the Create dialog box, enter an ID and click OK.

Identifying the Sampled Flowsheet Variables

For each sensitivity block you must identify the flowsheet variables and assign them variable names. You can either tabulate these variables or use them in Fortran expressions to compute tabulated results. The variable name identifies the flowsheet variable on other sensitivity sheets.

Use the Define sheet to identify a flowsheet variable and assign it a variable name. When completing a Define sheet, specify the variables on the Variable Definition dialog box. The Define sheet shows a concise summary of all the accessed variables, but you cannot modify the variables on the Define sheet.

On the Define sheet:

1. To create a new variable, click the New button.

   – or –

   To edit an existing variable, select a variable and click the Edit button.
2. Type the name of the variable in the Variable Name field.

   If you are editing an existing variable and want to change the variable name, click the right mouse button on the Variable Name field. On the popup menu, click Rename. A variable name must:

   - Be six characters or less for a scalar variable
   - Be five characters or less for a vector variable
   - Start with an alphabetic character (A – Z)
   - Have subsequent alphanumeric characters (A – Z, 0 – 9)
   - Not begin with IZ or ZZ
3. In the Category frame, use the option button to select the variable category.
4. In the Reference frame, select the variable type from the list in the Type field.

   Aspen Plus displays the other fields necessary to complete the variable definition.
5. Click Close to return to the Define sheet.

   For more information on accessing variables, see Chapter 18.

   Tips Use the Delete button to quickly delete a variable and all of the fields used to define it. Use the Edit button to modify the definition of a variable in the Variable Definition dialog box.

For more information about accessing flowsheet variables, see Chapter 18. For more information about using the Define sheet to identify flowsheet variables, see Chapter 19.

Identifying Manipulated Flowsheet Variables

Use the Vary sheet to identify the flowsheet variables to vary in generating a table. You can only vary block input variables, process feed stream variables, and other input variables. You must specify values, or a range of values, for the varied variables.

You can manipulate integer variables, such as the feed location of a distillation column. You can specify up to five manipulated variables.

To identify manipulated variables and specify values:

1. On the Sensitivity Input form, click the Vary sheet.
2. In the Variable Type field, select a variable type.

   Aspen Plus takes you to the remaining fields necessary to uniquely identify the flowsheet variable.
3. Specify a list or range of values for the manipulated variable. You can enter one of the following:
   - List of values
   - Lower limit, Upper limit, and number of equally spaced points (# Points)
   - Lower limit, Upper limit, and increment between points (Incr)

   You can enter either a constant or a Fortran expression.
4. You have the option of labeling the varied variables for the report and the Results Summary sheet. Use the Line1 through Line4 fields to define these labels.
5. To identify additional variables, select New from the list in the Variable Number field. Repeat Steps 2 through 5.

Aspen Plus generates one row of the table for each combination of varied variable values. The number of possible combinations can be large, resulting in excessive computer time and storage requirements. For example, 10 points for each of the maximum of five variables would result in 100,000 evaluations of the sensitivity block loop.

Each manipulated variable must already have been entered as an input specification, or it must have a default value.

Defining Tabulated Variables

Use the Tabulate sheet for defining the results you want Aspen Plus to tabulate, and supplying column headings.

To define tabulated variables:

1. On the Sensitivity Input form, click the Tabulate sheet.

2. In the Column Number field, enter a column number.
3. In the Tabulated Variable or Expression field, enter a variable name or Fortran expression.

   Aspen Plus tabulates the variable, or the result of the expression, for each combination of manipulated variables.

   To ensure that you enter accurate variable names, click the right mouse button. In the popup menu, click Variable List. The Defined Variable List window appears. You can drag and drop the variables from the Defined Variable List to the Fortran sheet.
4. To enter optional labels, click the Table Format button. In the first four rows, supply column labels for any or all of the columns of tabulated results.
5. Use the two Unit Labels rows to enter units labels for the tabulated results.
6. If the tabulated results expression is entered as a single variable name on the Specification sheet, Aspen Plus generates unit labels automatically.
7. Click Close to close the Table Format dialog box.
8. Repeat Steps 2 through 6 until you define all the results you want to tabulate. There is no limit.

Reinitializing Blocks and Streams

By default, Aspen Plus begins the calculations for a new row using the results of the previous row. If blocks or recycle loops fail to converge for some rows, you can specify that the calculations are to be reinitialized for each row.

Reinitializing Blocks

To reinitialize blocks:

1. On the Sensitivity Input form, select the Optional tab.
2. In the Blocks to be Reinitialized field, select either Include Specified Blocks or Reinitialize All Blocks.
3. If you choose Include Specified Blocks, select the unit operation blocks and/or the convergence blocks to be reinitialized.

Reinitializing Streams

To reinitialize streams:

1. On the Sensitivity Input form, select the Optional tab.

2. On the Streams To Be Reinitialized field select either Include Specified Streams or Reinitialize All Streams.
3. If you choose Include Specified Streams, select the streams to be reinitialized.

Entering Optional Fortran Statements

You have the option of entering Fortran statements to compute tabulated results and the varied variable range. Any variable computed by a Fortran statement can be used in expressions on the Tabulate and Vary sheets. Fortran statements are needed only if functions are too complex to enter on these sheets.

You can enter Fortran statements:

- On the Fortran sheet
- In your text editor (for example, Notepad), and then copy and paste them onto the Fortran sheet

Using the Sensitivity Input Fortran Sheet

To enter executable Fortran statements on the Fortran sheet:

1. On the Sensitivity Input form, click the Fortran sheet.
2. Review the rules and restrictions for in-line Fortran. For more information, see Chapter 19.
3. Enter your Fortran statements.

   To ensure that you enter accurate variable names, click the right mouse button. In the popup menu, click Variable List. The Defined Variable List window appears. You can drag and drop the variables from the Defined Variable List to the Fortran sheet.

Fortran Declarations

Enter Fortran declarations in the same way as executable Fortran statements, using the Declarations sheet instead of the Fortran sheet.

You can include any Fortran declaration in a Sensitivity block, including:

- COMMON definitions
- DIMENSION definitions
- Data type definitions (INTEGER and REAL)

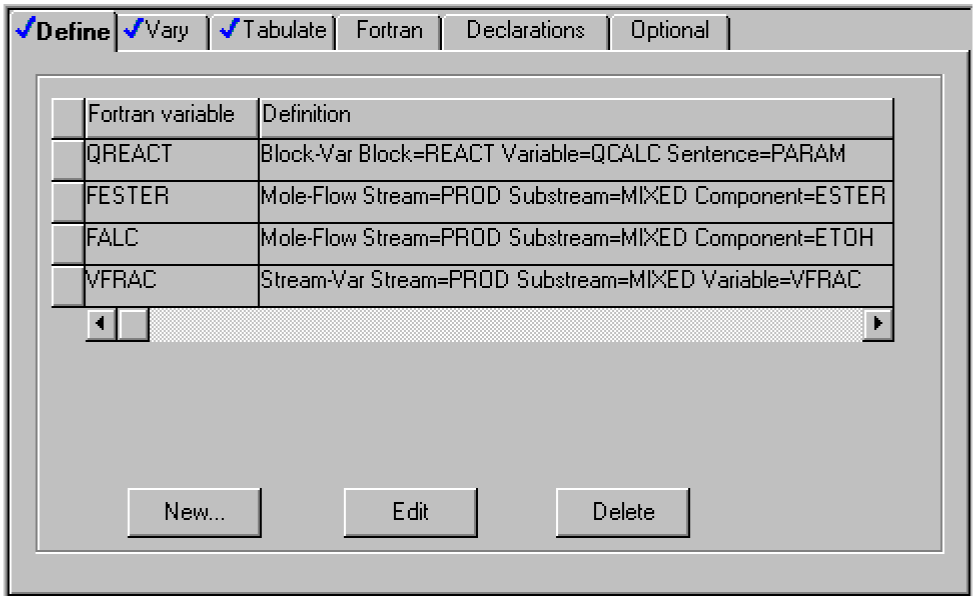
If a Fortran variable meets one of these criteria, you should place it in a COMMON:

- It is also used by another block.
- Its value must be retained from one iteration of a sensitivity block to another.

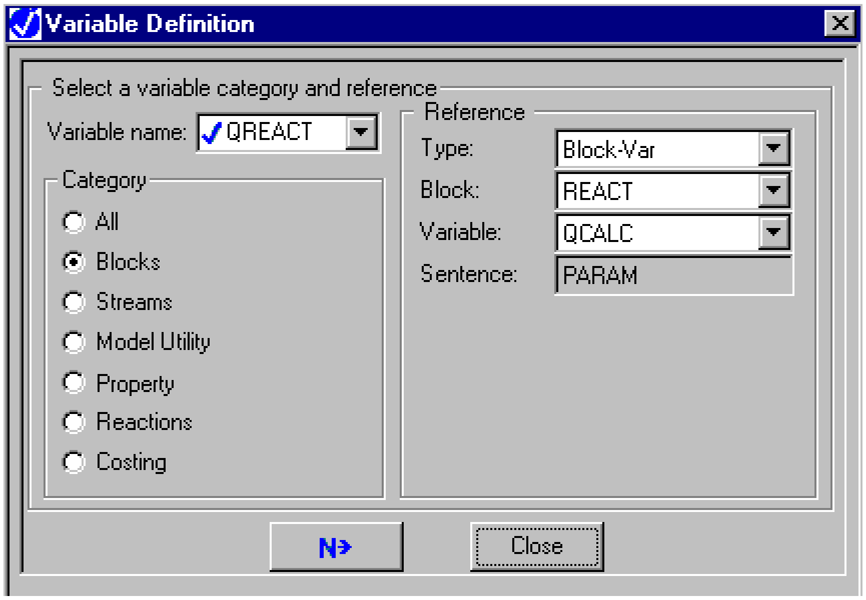
Fortran variables that you defined on the Define sheet should not be declared on the Declarations sheet.

Example for Tabulating Reaction Selectivity versus Reactor Temperature

Tabulate the effect of temperature in RGibbs block REACT on the selectivity of component ESTER versus ETOH in the reactor outlet. Assume that an initial specification for the temperature of block REACT has been entered on the RGibbs Setup Specifications sheet.



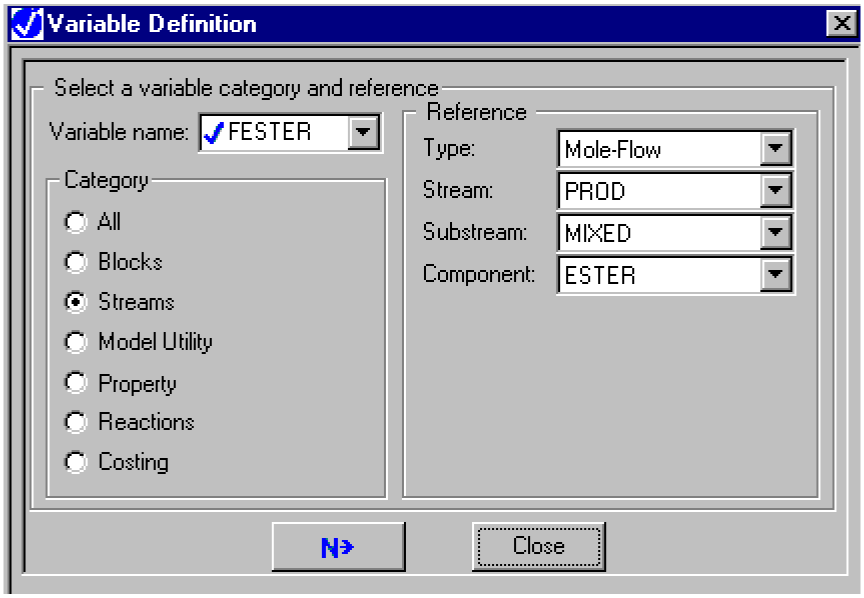
Fortran variable	Definition
QREACT	Block-Var Block=REACT Variable=QCALC Sentence=PARAM
FESTER	Mole-Flow Stream=PROD Substream=MIXED Component=ESTER
FALC	Mole-Flow Stream=PROD Substream=MIXED Component=ETOH
VFRAC	Stream-Var Stream=PROD Substream=MIXED Variable=VFRAC



Variable name: QREACT

Category:
○ All
● Blocks
○ Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

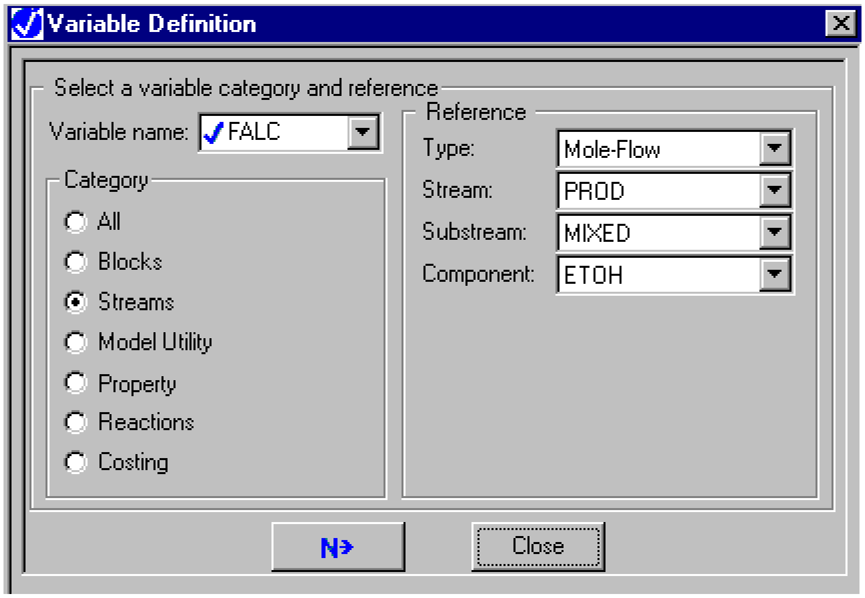
Type: Block-Var
Block: REACT
Variable: QCALC
Sentence: PARAM



Variable name: FESTER

Category:
○ All
○ Blocks
● Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

Type: Mole-Flow
Stream: PROD
Substream: MIXED
Component: ESTER



Variable Definition

Select a variable category and reference

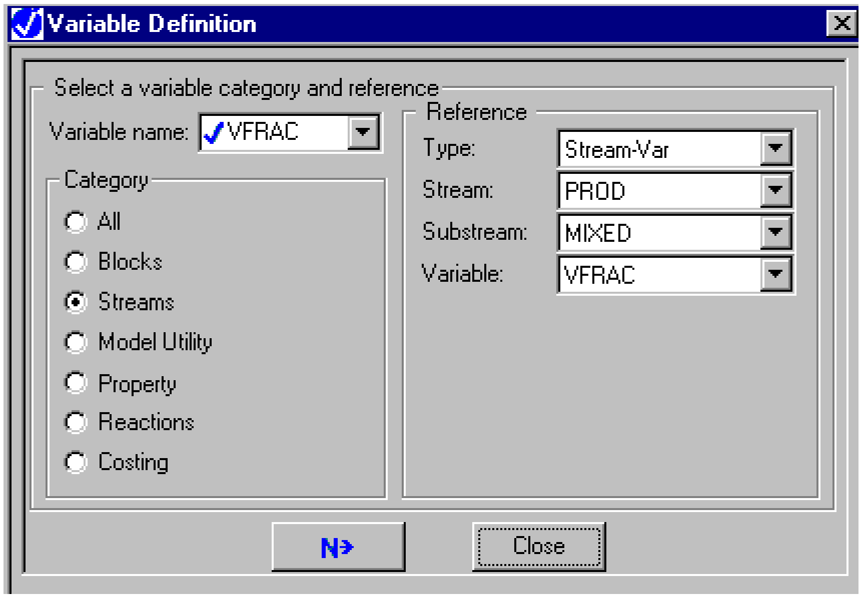
Variable name: FALC

Category

○ All
○ Blocks
● Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

Reference

Type: Mole-Flow
Stream: PROD
Substream: MIXED
Component: ETOH



Variable Definition

Select a variable category and reference

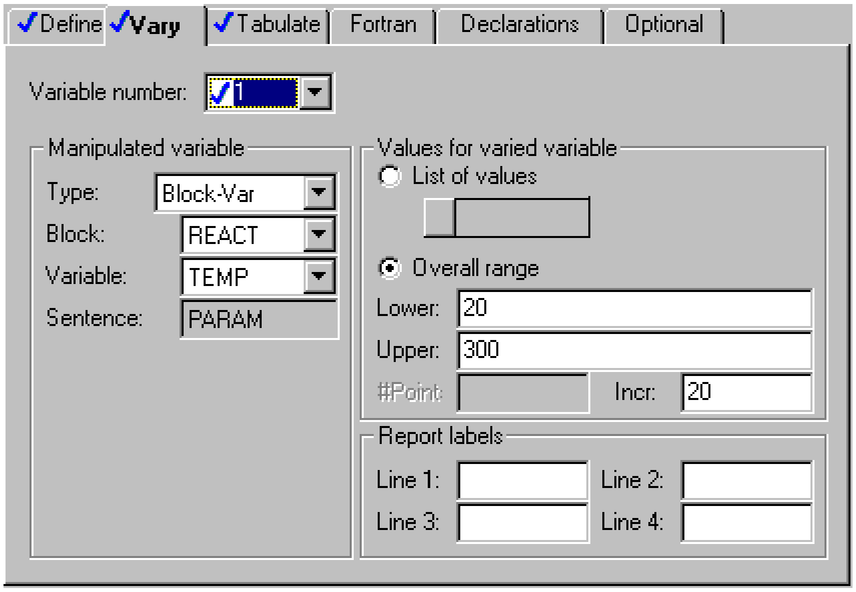
Variable name: VFRAC

Category

○ All
○ Blocks
● Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

Reference

Type: Stream-Var
Stream: PROD
Substream: MIXED
Variable: VFRAC



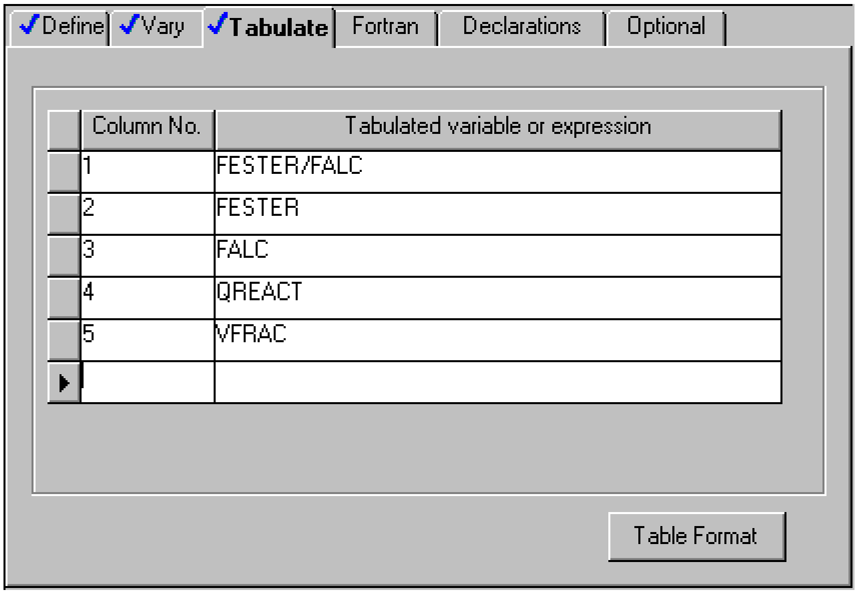
Variable number: ✓1

Type: Block-Var
Block: REACT
Variable: TEMP
Sentence: PARAM

○ List of values
● Overall range
Lower: 20
Upper: 300
#Point:
Incr: 20

Line 1:
Line 2:
Line 3:
Line 4:

The selectivity which is the ratio of FESTER to FALC can be entered as a Fortran expression FESTER/FALC on the Tabulate sheet.



Column No.	Tabulated variable or expression
1	FESTER/FALC
2	FESTER
3	FALC
4	QREACT
5	VFRAC

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21 Design Specifications: Feedback Control

Use design specifications as feedback controllers in your simulation. This chapter describes:

- What are design specifications?
- Creating design specifications
- Specifying targeted variables
- Specifying manipulated variables
- Optional Fortran statements

About Design Specifications

A design specification sets the value of a variable that Aspen Plus would otherwise calculate. For example, you may want to specify a product stream purity or the permissible amount of an impurity in a recycle stream. For each design specification, you identify a block input variable, process feed stream variable, or other simulation input to be manipulated (adjusted) to meet the specification. For example, you might manipulate a purge rate to control the level of impurities in a recycle stream. Design specifications can be used to simulate the steady state effect of a feedback controller.

When you use a design specification, you specify a desired value for a flowsheet variable or some function of flowsheet variables. The flowsheet variables used in a design specification are called sampled variables. For each design specification, you must also select a block input variable or process feed stream variable to be adjusted to satisfy the design specification. This variable is called the manipulated variable.

The design specification achieves its objective by manipulating an input variable specified by the user. Quantities that are calculated during the simulation should not be varied directly. For example, the stream flow rate of a recycle stream cannot be varied; however, the split fraction of an FSplit block where the recycle stream is an outlet can be varied. A design specification can only manipulate the value of one input variable.

Design specifications create loops that must be solved iteratively. By default Aspen Plus generates and sequences a convergence block for each design specification. You can override the default by entering your own convergence specifications. For a complete discussion of design specification convergence, see Chapter 17.

The value of the manipulated variable that is provided in the Stream or Block input is used as the initial estimate. Providing a good estimate for the manipulated variable will help the design specification converge in fewer iterations. This is especially important for large flowsheets with several interrelated design specifications.

The objective of the specification is that it equals the calculated value (Specified Value - Calculated Value = 0). The specification can be any valid Fortran expression involving one or more flowsheet quantities. Specifications must also have a tolerance within which the objective function relation must be satisfied. Therefore, the actual equation that must be satisfied is

$$| \text{Specified Value} - \text{Calculated Value} | < \text{Tolerance}$$

There are no results associated directly with a specification other than whether the objective function equation was satisfied or not. The final value of the manipulated an/or sampled variables can be viewed directly on the appropriate Stream or Block results sheets. The summary and iteration history of the Convergence block can be found by selecting the Results sheet of the appropriate Convergence block.

Defining a Design Specification

There are five steps involved in defining a design specification:

1. Creating the design specification
2. Identifying the sampled flowsheet variables used in the specification.
3. Specifying the target value for a sampled variable or some function of sampled variables and a tolerance.
4. Identifying a simulation input variable to be adjusted to achieve the target value, and specifying the limits within which it can be adjusted.

5. Entering optional Fortran statements.

Subsequent sections of this chapter describe each of these steps.

Creating a Design Specification

To create a design specification:

1. From the Data menu, point to Flowsheeting Options, then Design Specs.

   In the Design Specification Object Manager, click New.
2. In the Create New ID dialog box, enter an ID or accept the default, and click OK.

   The following sections describe how to complete the required sheets.

Identifying Sampled Flowsheet Variables

Use the Flowsheeting Options Design Spec Define sheet to identify the flowsheet variables used in the design specification and assign them variable names. The variable name identifies the flowsheet variable on other design specification sheets.

Use the Define sheet to identify a flowsheet variable and assign it a variable name. When completing a Define sheet, specify the variables on the Variable Definition dialog box. The Define sheet shows a concise summary of all the accessed variables, but you cannot modify the variables on the Define sheet.

On the Define sheet:

1. To create a new variable, click the New button.

   or

   To edit an existing variable, select a variable and click the Edit button.
2. Type the name of the variable in the Variable Name field. If you are editing an existing variable and want to change the variable name, click the right mouse button on the Variable Name field. On the popup menu, click Rename. A variable name must:
   - Be six characters or less for a scalar variable
   - Be five characters or less for a vector variable
   - Start with an alphabetic character (A – Z)
   - Have subsequent alphanumeric characters (A – Z, 0 – 9)
   - Not begin with IZ or ZZ
3. In the Category frame, use the option button to select the variable category.

4. In the Reference frame, select the variable type from the list in the Type field.

   Aspen Plus displays the other fields necessary to complete the variable definition.
5. Click Close to return to the Define sheet.

See Chapter 18, Accessing Flowsheet Variables for more information on accessing variables.

Tip Use the Delete button to quickly delete a variable and all of the fields used to define it.

Tip Use the Edit button to modify the definition of a variable in the Variable Definition dialog box.

Entering the Design Specification

To enter the design specification:

1. On the Design Spec form, click the Spec sheet.
2. In the Spec field, enter the target variable or Fortran expression.
3. In the Target field, specify the target value as a constant or Fortran expression.
4. In the Tolerance field, enter the specification tolerance as a constant or Fortran expression.

The design specification is:

Spec expression = Target expression

The design specification is converged when:

– Tolerance < Spec expression – Target expression < Tolerance

If you need to enter more complex Fortran than can be handled in a single expression, you can enter additional Fortran statements. See Entering Optional Fortran Statements, this chapter.

Tip To ensure that you enter accurate variable names, click the right mouse button on the Spec, Target, or Tolerance field. In the popup menu, click Variable List. The Defined Variable List window appears. You can drag and drop the variables from the Defined Variable List to the Spec sheet.

Identifying the Manipulated Variable

Use the Vary sheet to identify the manipulated variable and specify its limits. The limits for manipulated variables can be constants or functions of flowsheet variables.

To identify the manipulated variable and specify limits:

1. On the Design Spec form, click the Vary sheet
2. In the Type field, select a variable type.

   Aspen Plus takes you to the remaining fields necessary to uniquely identify the flowsheet variable.
3. In the Lower field, enter a constant or Fortran expression as the lower limit for the manipulated variable.
4. In the Upper field, enter a constant or Fortran expression as the upper limit for the manipulated variable.

You must have already entered the manipulated variable as an input specification, or it must have a default value. The initial guess used for the manipulated variable is this specification or the default. You cannot manipulate integer block input variables, such as the feed location of a distillation column.

If the design specification cannot be met because the solution is outside the limit range, Aspen Plus chooses the limit that most closely meets the specification.

Entering Optional Fortran Statements

You have the option of entering any Fortran statements needed to compute the design specification terms or manipulated variable limits. Any variable that is computed by the Fortran statements can be used in the expressions on the Spec and Vary sheets. Fortran statements are needed only if the functions involved are too complex to enter on the Spec and Vary sheets.

You can enter Fortran statements:

- On the Fortran sheet
- In your text editor (for example, Notepad), and then copy and paste them onto the Fortran sheet

Enter Fortran declarations in the same way as executable Fortran statements, using the Declarations sheet instead of the Fortran sheet.

You can include any Fortran declarations in a Fortran block, such as:

- Include statements
- COMMON definitions
- DIMENSION definitions

- Data type definitions (INTEGER and REAL)

If a Fortran variable meets one of these criteria, you should place it in a COMMON:

- It is also used by another block.
- Its value must be retained from one iteration of a Fortran block to another.

Fortran variables that you defined on the Specification sheet should not be declared on the Declarations sheet.

Using the Fortran Sheet

To enter executable Fortran statements on the Fortran sheet:

1. On the Design Spec form, click the Fortran sheet.
2. Use Help to review rules and restrictions for in-line Fortran.
3. Enter your Fortran statements.

   To ensure that you enter accurate variable names, click the right mouse button. In the popup menu, click Variable List. The Defined Variable List window appears. You can drag and drop the variables from the Defined Variable List to the Fortran sheet.

Troubleshooting Design Specifications

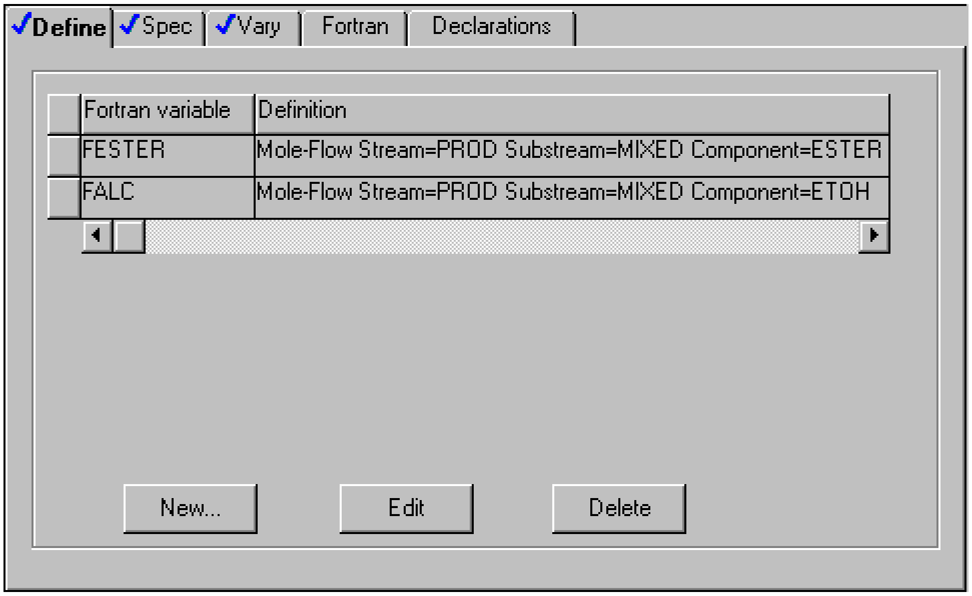
If the objective function was not satisfied, there are a number of options to consider:

- Check to see that the manipulated variable is not at its lower or upper bound.
- Verify that a solution exists within the bounds specified for the manipulated variable, perhaps by performing a sensitivity analysis.
- Check to ensure that the manipulated variable does indeed affect the value of the sampled variable.
- Try providing a better starting estimate for the value of the manipulated variable.
- Narrowing the bounds of the manipulated variable or loosening the tolerance on the objective function might help convergence.
- Try changing the characteristics of the Convergence block associated with the design specification (step size, number of iterations, etc.)
- Make sure that the objective function does not have a flat region within the range of the manipulated variable.

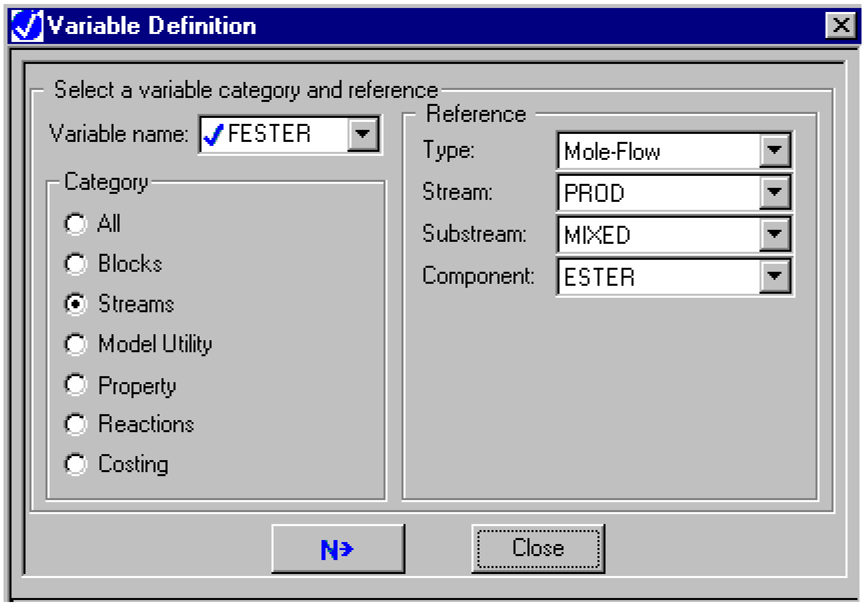
Example for Feedback Control of Reactor Selectivity

Manipulate the temperature of RGibbs block REACT to control the selectivity of component ESTER versus ETOH at a value of 2.50 +/- 0.01. This example assumes that temperature was specified for block REACT on the RGibbs Setup Specification sheet. The RGibbs specification becomes the initial estimate for the design specification.

- The molar flow rate of ESTER and of ETOH in stream PROD are the sample variables. These variables are called FESTER and FALC, respectively.
- The design specification is FESTER/FALC = 2.50.
- The design specification is satisfied when |FESTER/FALC -2.50| < 0.01.
- Fortran expressions such as FESTER/FALC can be used in any part of the specification expression: the spec, the target or the tolerance.
- The reactor temperature is the manipulated variable. The design specification convergence block will find the reactor temperature that makes FESTER/FALC=2.5.
- The temperature is specified in the reactor block just as if there were no design specification. The specified value is the initial estimate used by the design specification convergence block.
- The design specification convergence block will not try a temperature less than 50F or greater than 150F, even if the solution to the objective function lies outside this range. The limits become alternative specifications if the design specification cannot be achieved. The initial estimate entered in the reactor block lies within these limits.
- You do not have to specify convergence of the design specification. Aspen Plus will automatically generate a convergence block to converge the specification.



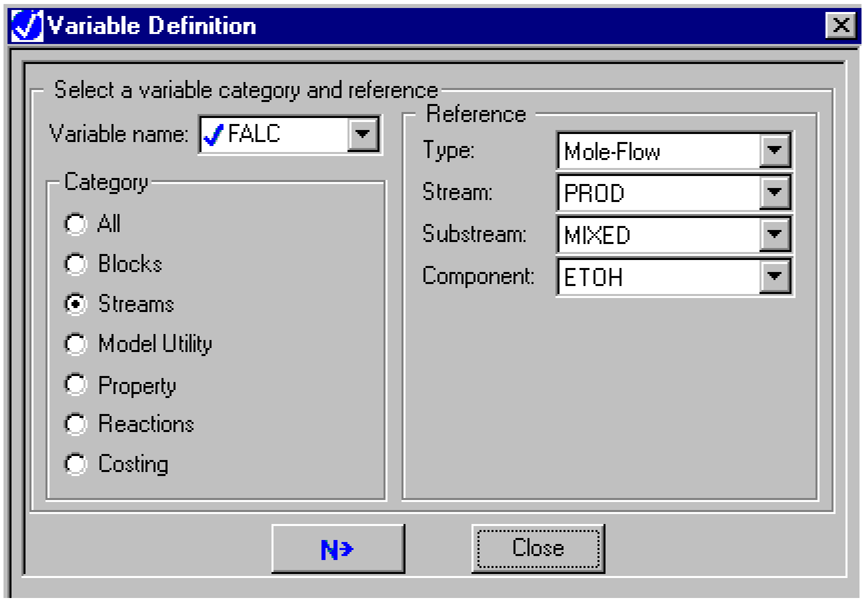
Fortran variable	Definition
FESTER	Mole-Flow Stream=PROD Substream=MIXED Component=ESTER
FALC	Mole-Flow Stream=PROD Substream=MIXED Component=ETOH



Variable name: FESTER

○ All
○ Blocks
● Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

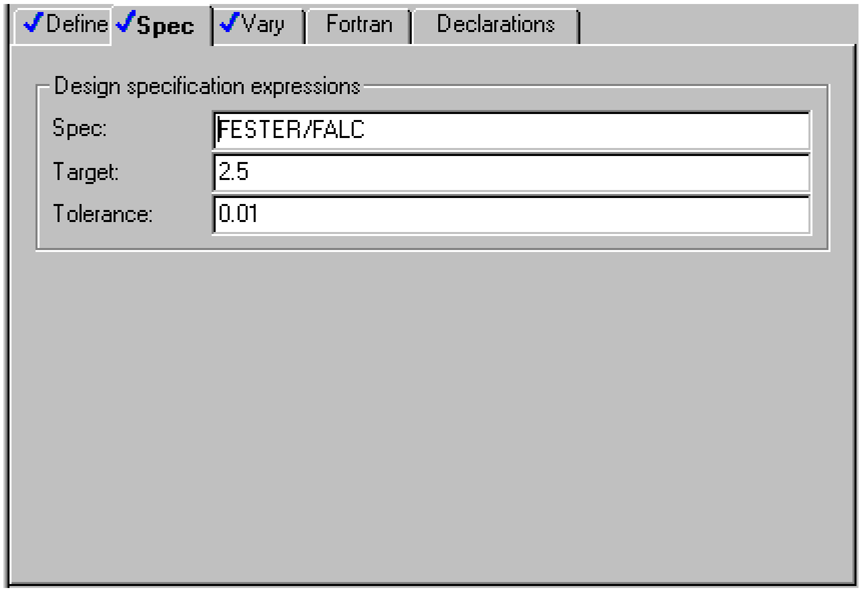
Type: Mole-Flow
Stream: PROD
Substream: MIXED
Component: ESTER



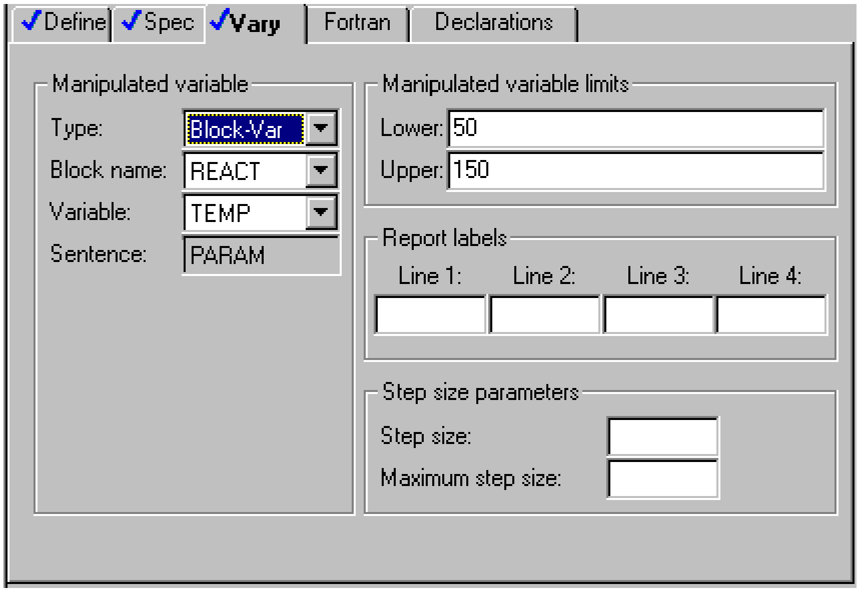
Variable name: FALC

○ All
○ Blocks
● Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

Type: Mole-Flow
Stream: PROD
Substream: MIXED
Component: ETOH



Spec: FESTER/FALC
Target: 2.5
Tolerance: 0.01



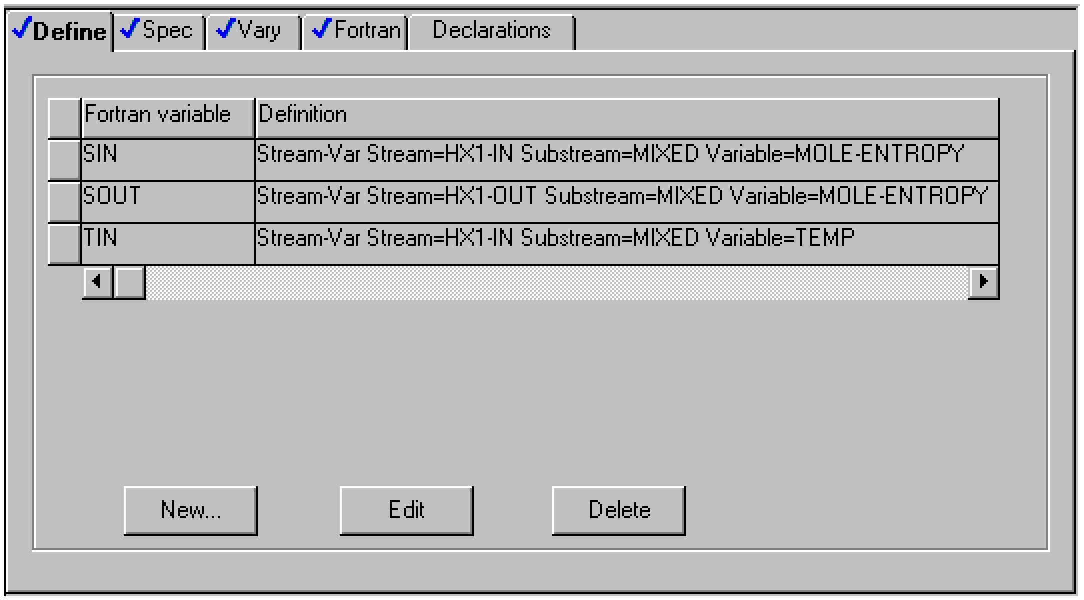
Type: Block-Var
Block name: REACT
Variable: TEMP
Sentence: PARAM
Lower: 50
Upper: 150

Example for Design Specification with Variable Tolerance and Limits

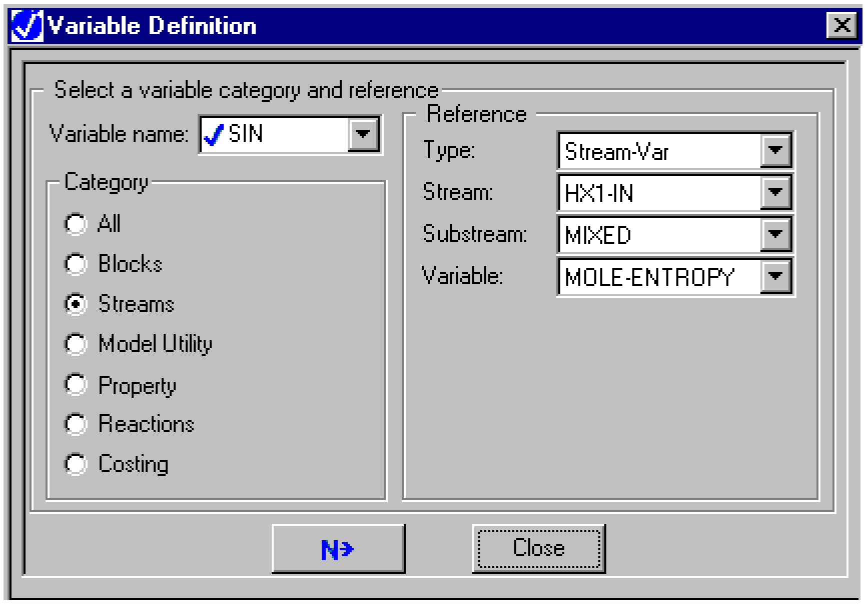
A design specification designates that the inlet and outlet entropies of a Heater block HX1 are equal. The temperature of HX1 is chosen as the manipulated variable. Temperature limits cannot be set a priori, but it is known that the isentropic temperature will be within 75°F of the inlet temperature. The tolerance for the specification is a function of the entropy.

- The inlet and outlet entropy and the inlet temperature of the block HX1 are the sample variables. The entropy of the inlet stream HX1-IN is called SIN. The outlet entropy of the outlet stream HX1-OUT is called SOUT. The temperature of stream HX1-IN is called TIN.

- The design specification sets the inlet entropy SOUT equal to the inlet entropy SIN.
- The tolerance is specified as the variable TOL. TOL is specified as 0.0001 times the absolute value of the entropy of the inlet stream SIN on the Design Spec Fortran sheet.
- The design specification is satisfied when |SOUT - SIN| < TOL.
- The temperature is specified in the Heater block just as if there were no design specification. The specified value is the initial estimate used by the design specification convergence block.
- The design specification convergence block will not try a temperature less than the inlet temperature TIN - 75F or greater than TIN + 75F, even if the solution to the objective function lies outside this range. The limits become alternative specifications if the design specification cannot be achieved. The initial estimate entered in the reactor block lies within these limits.
- You do not have to specify convergence of the design specification. Aspen Plus will automatically generate a convergence block to converge the specification.



Fortran variable	Definition
SIN	Stream-Var Stream=HX1-IN Substream=MIXED Variable=MOLE-ENTROPY
SOUT	Stream-Var Stream=HX1-OUT Substream=MIXED Variable=MOLE-ENTROPY
TIN	Stream-Var Stream=HX1-IN Substream=MIXED Variable=TEMP



Variable Definition

Select a variable category and reference

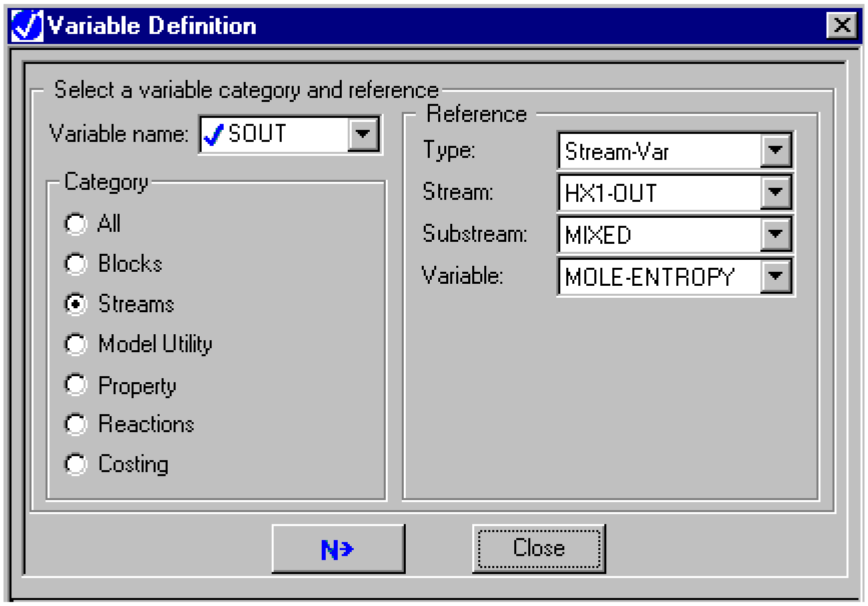
Variable name: SIN

Category

○ All
○ Blocks
● Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

Reference

Type: Stream-Var
Stream: HX1-IN
Substream: MIXED
Variable: MOLE-ENTROPY



Variable Definition

Select a variable category and reference

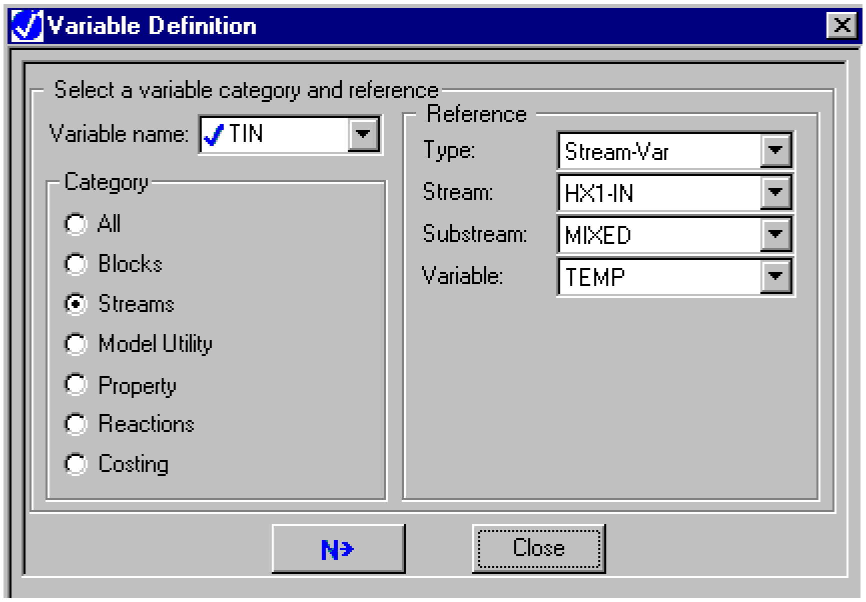
Variable name: SOUT

Category

○ All
○ Blocks
● Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

Reference

Type: Stream-Var
Stream: HX1-OUT
Substream: MIXED
Variable: MOLE-ENTROPY



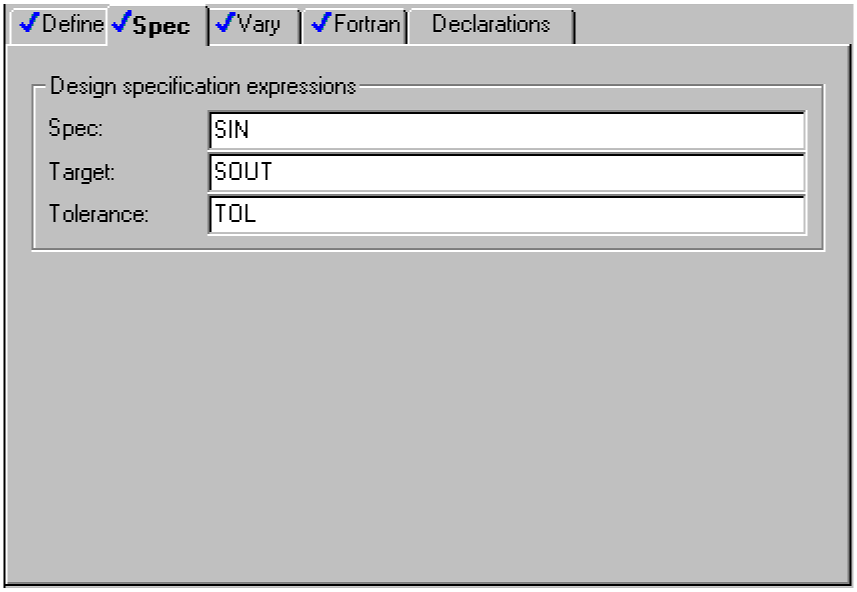
Variable Definition

Select a variable category and reference

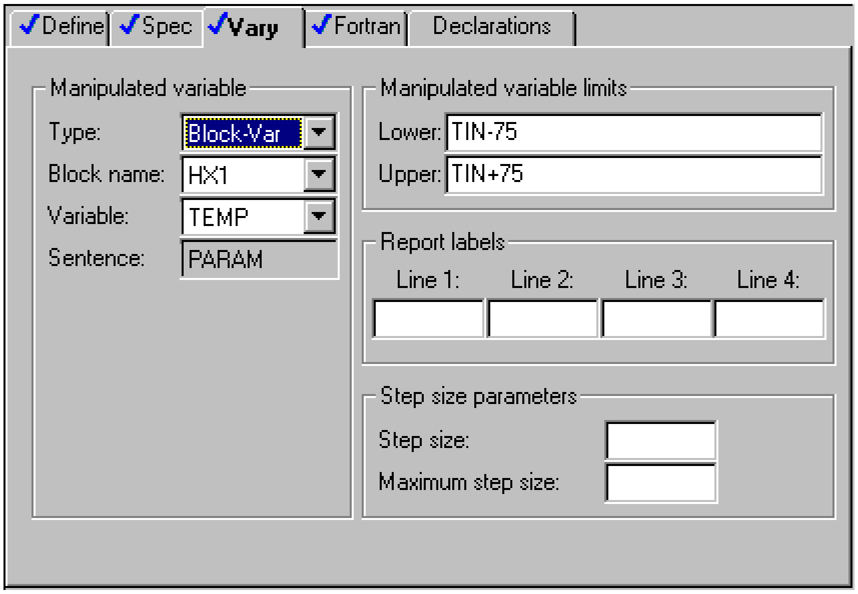
Variable name: TIN

Category
- ○ All
- ○ Blocks
- ● Streams
- ○ Model Utility
- ○ Property
- ○ Reactions
- ○ Costing

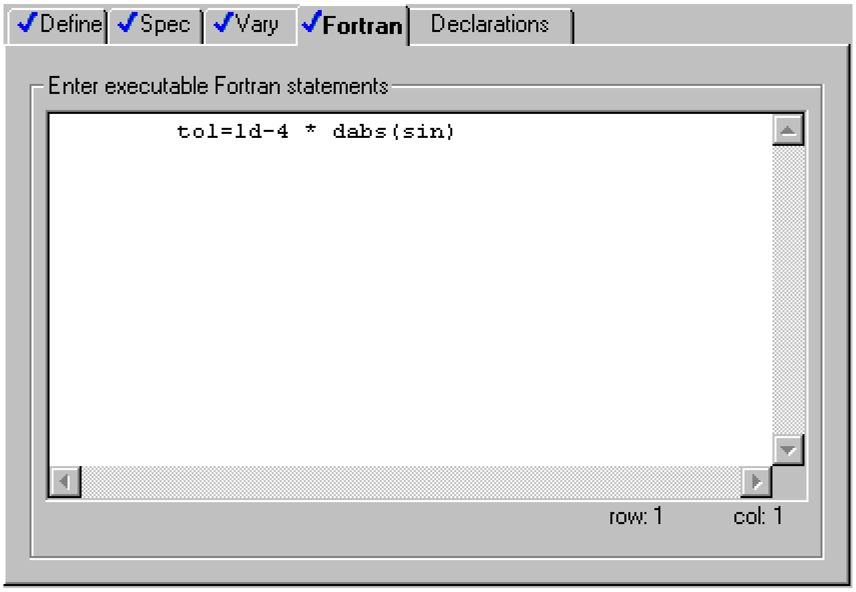
Reference
Type: Stream-Var
Stream: HX1-IN
Substream: MIXED
Variable: TEMP



Design specification expressions
Spec: SIN
Target: SOUT
Tolerance: TOL



Type: Block-Var
Block name: HX1
Variable: TEMP
Sentence: PARAM
Lower: TIN-75
Upper: TIN+75

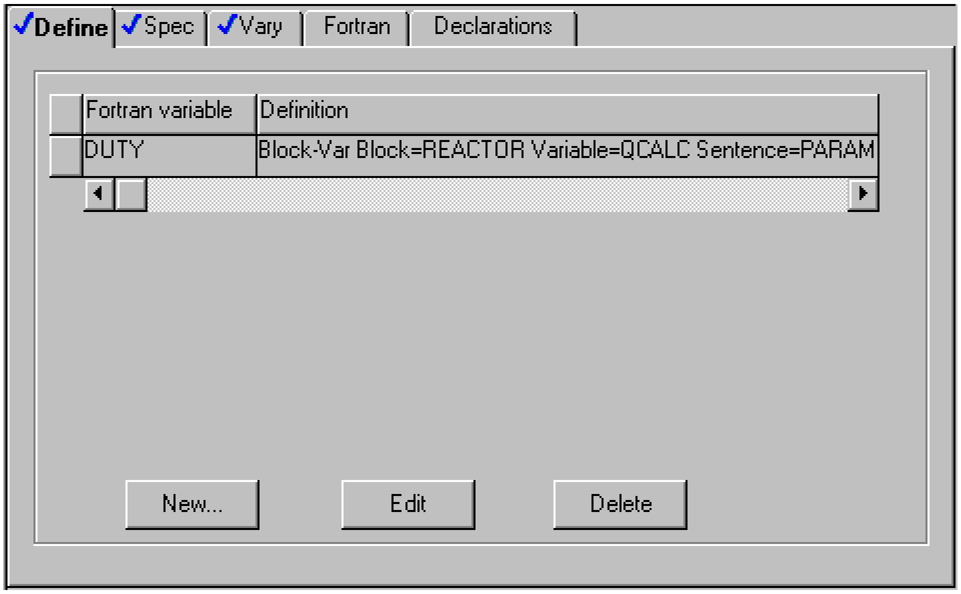


```
         tol=1d-4 * dabs(sin)
```

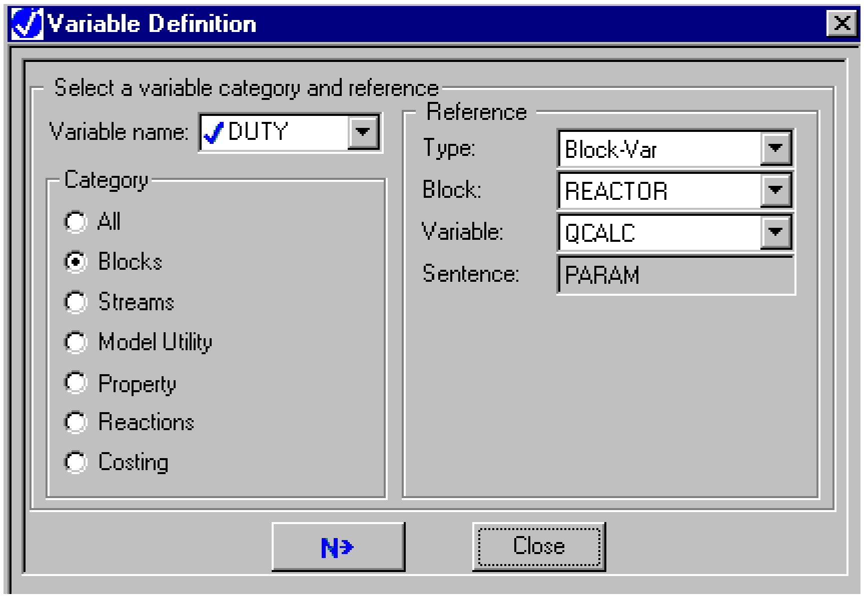
Example for Adjusting the Standard Enthalpy of Formation to Achieve a Desired Heat of Reaction

The heat of reaction for the hydrogenation of ethylene is known to be -32700 cal/mol at 298 K. Aspen Plus predicts a value of -32570. Since it is possible to access physical property parameters (see Chapter 19, Accessing Variables), a design specification is used to adjust the Standard Enthalpy of Formation to achieve the desired heat of reaction.

In Aspen Plus, the heat of reaction is calculated as the difference in enthalpy of the pure components. Since the Standard Enthalpy of Formation (pure component parameter DHFORM) is used to calculate vapor and liquid enthalpies, adjusting DHFORM will similarly adjust the heat of reaction.



Fortran variable	Definition
DUTY	Block-Var Block=REACTOR Variable=QCALC Sentence=PARAM



Select a variable category and reference

Variable name: DUTY

Category
- ○ All
- ● Blocks
- ○ Streams
- ○ Model Utility
- ○ Property
- ○ Reactions
- ○ Costing

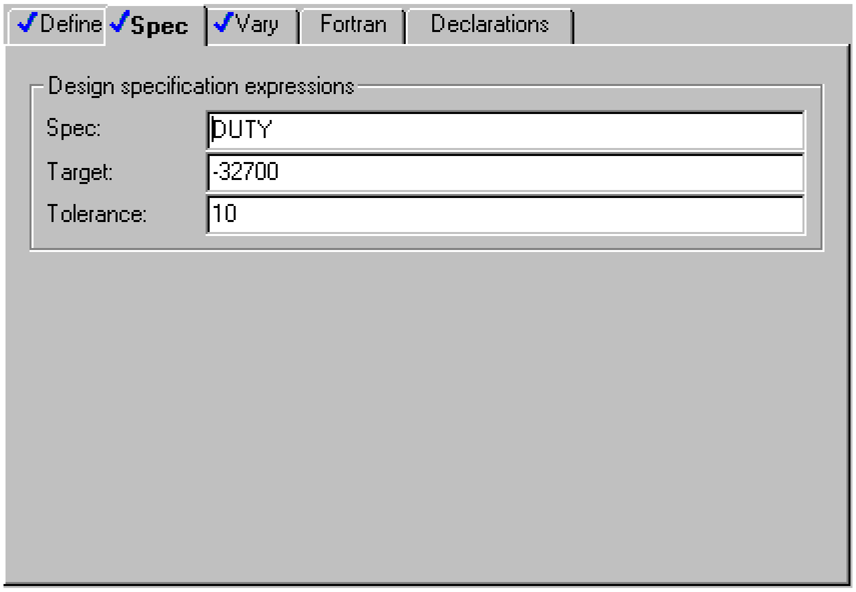
Reference

Type: Block-Var

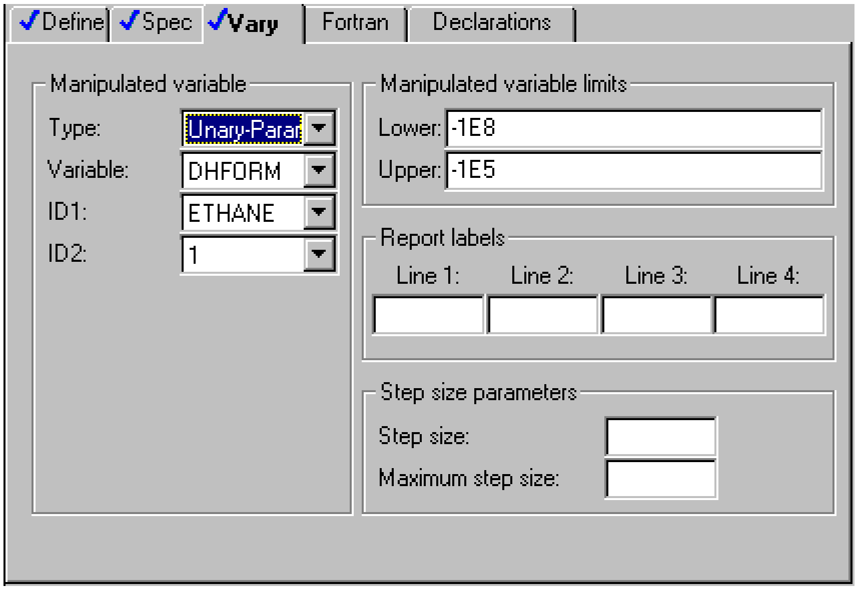
Block: REACTOR

Variable: QCALC

Sentence: PARAM



Spec: DUTY
Target: -32700
Tolerance: 10



Type: Unary-Parar
Variable: DHFORM
ID1: ETHANE
ID2: 1
Lower: -1E8
Upper: -1E5

❖ ❖ ❖ ❖

22 Optimization

This chapter includes information on:

- About Optimization
- Recommended Procedure for Optimization
- Defining an Optimization Problem
- About Constraints
- Entering Optional Fortran Statements
- Fortran Declarations
- Convergence of Optimization Problems
- Troubleshooting Optimization Problems

About Optimization

Use optimization to maximize or minimize a user-specified objective function by manipulating decision variables (feed stream, block input, or other input variables).

The objective function can be any valid Fortran expression involving one or more flowsheet quantities. The tolerance of the objective function is the tolerance of the convergence block associated with the optimization problem.

You have the option of imposing equality or inequality constraints on the optimization. Equality constraints within an optimization are similar to design specifications. The constraints can be any function of flowsheet variables computed using Fortran expressions or in-line Fortran statements. You must specify the tolerance of the constraint.

Tear streams and the optimization problem can be converged simultaneously or separately. If they are converged simultaneously, the tear stream is treated as an additional constraint.

Convergence of Optimization Problems

Aspen Plus solves optimization problems iteratively. By default Aspen Plus generates and sequences a convergence block for the optimization problem. You can override the convergence defaults, by entering convergence specifications on Convergence forms. Use the SQP and Complex methods to converge optimization problems. See Chapter 17 for a complete discussion of optimization convergence.

The value of the manipulated variable that is provided in the Stream or Block input is used as the initial estimate. Providing a good estimate for the manipulated variable helps the optimization problem converge in fewer iterations. This is especially important for optimization problems with a large number of varied variables and constraints.

There are no results associated directly with an optimization problem, except the objective function and the convergence status of the constraints. You can view the final value of the manipulated and/or sampled variables either directly on the appropriate Stream or Block results sheets or summarized on the Results Manipulated Variables sheet of the convergence block. To find the summary and iteration history of the convergence block, select the Results form of the appropriate Convergence block.

Recommended Procedure for Optimization

Optimization problems can be difficult to formulate and converge. It is important to have a good understanding of the simulation problem before adding the complexity of optimization.

The recommended procedure for creating an optimization problem is:

1. Start with a simulation (instead of starting with optimization). There are a number of reasons for this approach:
    - It is easier to detect flowsheet errors in a simulation.
    - You can determine reasonable specifications.
    - You can determine a reasonable range of decision variables.
    - You can get a good estimate for the tear streams.
2. Perform sensitivity analysis before optimization, to find appropriate decision variables and their ranges.
3. Evaluate the solution using sensitivity analysis, to find out if the optimum is broad or narrow.

Defining an Optimization Problem

Define an optimization problem by:

1. Creating the optimization problem.
2. Identifying the sampled flowsheet variables used in the objective function.
3. Specifying the objective function for a sampled variable, or some function of sampled variables, and identify the constraints associated with the problem.
4. Identifying the simulation input variables to be adjusted to maximize or minimize the objective function, and specify the limits within which they can be adjusted.
5. Entering optional Fortran statements.
6. Defining the constraints for the optimization problem.

Creating an Optimization Problem

To create an optimization problem:

1. From the Data menu, point to Model Analysis Tools, then Optimization.
2. In the Optimization Object Manager, click New.
3. In the Create New ID dialog box, enter an ID (or accept the default ID) and click OK.

Identifying Sampled Flowsheet Variables

Use the Model Analysis Optimization Define sheet to identify the flowsheet variables used in setting up the optimization problem, and assign them variable names. The variable name identifies the flowsheet variable that you can use when defining the objective function, specifying bounds for the manipulated vairables, or writing Fortran statements.

Use the Define sheet to identify a flowsheet variable and assign it a variable name. When completing a Define sheet, specify the variables on the Variable Definition dialog box. The Define sheet shows a concise summary of all the accessed variables, but you cannot modify the variables on the Define sheet.

On the Define sheet:

1. To create a new variable, click the New button.

   or

   To edit an existing variable, select a variable and click the Edit button.
2. Type the name of the variable in the Variable Name field. If you are editing an existing variable and want to change the variable name, click the right mouse button on the Variable Name field. On the popup menu, click Rename. A variable name must:
   - Be six characters or less for a scalar variable
   - Be five characters or less for a vector variable
   - Start with an alphabetic character (A – Z)
   - Have subsequent alphanumeric characters (A – Z, 0 – 9)
   - Not begin with IZ or ZZ
3. In the Category frame, use the option button to select the variable category.
4. In the Reference frame, select the variable type from the list in the Type field.

   Aspen Plus displays the other fields necessary to complete the variable definition.
5. Click Close to return to the Define sheet.

See Chapter 18, Accessing Flowsheet Variables for more information on accessing variables.

Tip Use the Delete button to quickly delete a variable and all of the fields used to define it.

Tip Use the Edit button to modify the definition of a variable in the Variable Definition dialog box.

Entering the Objective Function

If any constraints are associated with the optimization, define them before you specify the Objective function. For more information, see Defining Constraints, this chapter.

To enter the objective function for the optimization problem and identify the constraints:

1. On the Optimization form, click the Objective & Constraints tab.
2. Select either Maximize or Minimize.

3. In the Objective Function field, enter the targeted variable or Fortran expression.

   To ensure that you enter accurate variable names, click the right mouse button. In the popup menu, click Variable List. The Defined Variable List window appears. You can drag and drop the variables from the Defined Variable List to the Objective Function field.
4. Select the constraints to be associated with the optimization, using the arrow buttons to move them from the Available Constraints list to the Selected Constraints list.

If you need to enter more complex Fortran than can be handled in a single expression, you can enter additional Fortran statements. For more information, see Entering Optional Fortran Statements, this chapter.

Identifying the Manipulated Variable

Use the Vary sheet to identify the manipulated variables and specify their limits. The limits for manipulated variables can be constants or functions of flowsheet variables.

To identify the manipulated variable and specify limits:

1. On the Optimization form, click the Vary tab.
2. In the Variable Number field, click on the down arrow and select <new>.
3. In the Type field, select a variable type.

   Aspen Plus takes you to the remaining fields necessary to uniquely identify the flowsheet variable. For more information on accessing variables, see Chapter 18.
4. In the Lower field, enter a constant or Fortran expression as the lower limit for the manipulated variable.
5. In the Upper field, enter a constant or Fortran expression as the upper limit for the manipulated variable.
6. You can label the decision variables for the report and the Results form. Use the Line 1 to Line 4 fields to define these labels.
7. Repeat steps 2 though 6 until you identify all manipulated variables.

You must have already entered the manipulated variable as an input specification, or it must have a default value. The initial guess used for the manipulated variable is either this specification or the default. You cannot manipulate integer block input variables, such as the feed location of a distillation column.

About Constraints

You can choose to specify equality and inequality constraints for optimization problems. Equality constraints are the same as design specifications in non-optimization problems. Supply an ID for each constraint you define. Constraint IDs identify constraints on the Optimization sheets.

Defining Constraints

Define a constraint by:

1. Creating the constraint.
2. Identifying the sampled flowsheet variables used in the constraint.
3. Specifying the constraint expression.
4. Ensuring the constraint has been selected on the Optimization Objective & Constraints sheet.

Creating Constraints

To create a constraint problem:

1. From the Data menu, point to Model Analysis Tools, then Constraint.
2. In the Constraint Object Manager, click New.
3. In the Create New ID dialog box, enter an ID (or accept the default ID) and click OK.

Identifying Sampled Flowsheet Variables for Constraints

Use the ModelAnalysis Constraint Define sheet to identify the flowsheet variables used in the optimization problem and assign them variable names. The variable name identifies the flowsheet variable that you can use on the Spec and Fortran sheets.

Use the Define sheet to identify a flowsheet variable and assign it a variable name. When completing a Define sheet, specify the variables on the Variable Definition dialog box. The Define sheet shows a concise summary of all the accessed variables, but you cannot modify the variables on the Define sheet.

On the Define sheet:

1. To create a new variable, click the New button.

   or

   To edit an existing variable, select a variable and click the Edit button.
2. Type the name of the variable in the Variable Name field. If you are editing an existing variable and want to change the variable name, click the right mouse button on the Variable Name field. On the popup menu, click Rename. A variable name must:
   - Be six characters or less for a scalar variable
   - Be five characters or less for a vector variable
   - Start with an alphabetic character (A – Z)
   - Have subsequent alphanumeric characters (A – Z, 0 – 9)
   - Not begin with IZ or ZZ
3. In the Category frame, use the option button to select the variable category.
4. In the Reference frame, select the variable type from the list in the Type field.

   Aspen Plus displays the other fields necessary to complete the variable definition.
5. Click Close to return to the Define sheet.

See Chapter 18, Accessing Flowsheet Variables for more information on accessing variables.

Tip Use the Delete button to quickly delete a variable and all of the fields used to define it.

Tip Use the Edit button to modify the definition of a variable in the Variable Definition dialog box.

Specifying the Constraint Expression

You need to specify the constraint as a function of the sampled variable and supply a tolerance on the constraint.

Constraint functions are defined as follows:

- For equality constraints:
- $-tolerance < expression1 - expression2 < tolerance$
- For less than or equal to inequality constraints:
- $expression1 - expression2 \leq tolerance$
- For greater than or equal to inequality constraints:
- $expression1 - expression2 \geq tolerance$

To specify a constraint:

1. On the Constraint form, click the Spec tab.
2. In the two Constraint expression specification fields, enter expression1 and expression2, as constants or Fortran expressions.

   To ensure that you enter accurate variable names, click the right mouse button. In the popup menu, click Variable List. The Defined Variable List window appears. You can drag and drop the variables from the Defined Variable List to the fields on the Spec form.
3. Select Equal to, Less than or equal to, or Greater than or equal to, for the specification.
4. In the Tolerance field, enter the constraint tolerance as a constant or as a Fortran expression.
5. If the constraint is a vector, check the This is a Vector Constraint box, and specify the elements of the vector that should be used.

If you need to enter more complex Fortran than can be handled in a single expression, you can enter additional Fortran statements on the Constraint Fortran sheet. (See Optional Fortran Statements, this chapter.)

Entering Optional Fortran Statements

You have the option of entering any Fortran statements needed to compute the optimization objective function terms or manipulated variable limits. Any variable computed by the Fortran statements can be used in the expressions on the following sheets:

- Optimization Objective & Constraint
- Optimization Vary
- Constraint Spec

Fortran statements are needed only if the functions involved are too complex to enter on these sheets.

You can enter Fortran statements:

- On the Fortran sheet
- In your text editor (for example, Notepad), and then copy and paste them onto the Fortran sheet.

Using the Fortran Sheet

To enter executable Fortran statements on the Fortran sheet:

1. On the Optimization or Constraint form, click the Fortran tab.
2. Review the rules and restrictions for in-line Fortran. For more information, see Chapter 19.
3. Enter your Fortran statements.

   To ensure that you enter accurate variable names, click the right mouse button. In the popup menu, click Variable List. The Defined Variable List window appears. You can drag and drop the variables from the Defined Variable List to the Fortran sheet.

Fortran Declarations

You enter Fortran declarations in the same way as executable Fortran statements, using the Declarations sheet instead of the Fortran sheet.

You can include any Fortran declarations in an optimization problem, including:

- COMMON definitions
- DIMENSION definitions
- Data type definitions (INTEGER and REAL)

If a Fortran variable meets one of these criteria, you should place it in a COMMON:

- It is also used by another block.
- Its value must be retained from one iteration of an optimization problem to another.

Fortran variables that you defined on the Define sheet should not be declared on the Declarations sheet.

Convergence of Optimization Problems

Algorithms for solving process optimization problems can be divided into two categories:

Path Method	Information
Feasible	Requires that tear streams and equality constraints (design specifications), if any, be converged at each iteration of the optimization.
Infeasible	Can converge tear streams, equality constraints, and inequality constraints simultaneously with the optimization problem.

Two optimization algorithms are available in Aspen Plus:

- The COMPLEX method
- The SQP method

For more information, see Chapter 17.

COMPLEX Method

The COMPLEX method uses the well-known Complex algorithm, a feasible path “black-box” pattern search. The method can handle inequality constraints and bounds on decision variables. Equality constraints must be handled as design specifications. You must use separate convergence blocks to converge any tear streams or design specifications.

The COMPLEX method frequently takes many iterations to converge, but does not require numerical derivatives. It has been widely used for all kinds of optimization applications for many years, and offers a well-established and reliable option for optimization convergence.

Sequential Quadratic Programming (SQP) Method

The SQP method is a state-of-the-art, quasi-Newton nonlinear programming algorithm. It can converge tear streams, equality constraints, and inequality constraints simultaneously with the optimization problem. The SQP method usually converges in only a few iterations but requires numerical derivatives for all decision and tear variables at each iteration.

The SQP method as implemented in Aspen Plus includes a novel feature: the tear streams can be partially converged using Wegstein, each optimization iteration and during line searches. This usually stabilizes convergence, and can reduce the overall number of iterations.

You can specify the number of Wegstein passes. Choosing a large value effectively makes SQP a feasible path (but not a black-box) method. The Aspen Plus default is to perform three Wegstein passes.

You can also use the SQP method as a black-box or partial black-box method, by converging tear streams and design specifications as an inside loop to the optimization problem (using separate Convergence blocks). This reduces the number of decision variables. The trade-off is the number of derivative evaluations, versus the time required per derivative evaluation. Whether SQP is the method of choice depends on your optimization problem.

The default optimization convergence procedure in Aspen Plus is to converge tear streams and the optimization problem simultaneously, using the SQP method.

Troubleshooting Optimization Problems

The convergence of an optimization problem can be sensitive to the initial values of the manipulated variables. The optimization algorithm only finds local maxima and minima in the objective function. Although it occurs rarely it is possible to obtain a different maximum or minimum in the objective function by starting at a different point in the solution space.

When an objective function is not satisfied, there are a number of options to consider:

1. Make sure the objective function does not have a flat region within the range of a manipulated variable. Avoid the use of objective functions and constraints that contain discontinuities.
2. Linearize the constraints to the extent possible.
3. If the error improves initially, but then levels off, the derivatives calculated are sensitive to step size. Some things to try are:
   - Tighten tolerances of unit operation and convergence blocks within the optimization convergence loop. The optimization tolerance should be equal to the square root of the block tolerances. For example, if the optimization tolerance is 10^{-3}, then the block tolerances should be 10^{-6}.
   - Adjust the step size for better accuracy. The step size should be equal to the square root of the inner tolerances.
   - Check to see that the manipulated variable is not at its lower or upper bound.

- Disable the Use Results from Previous Convergence Pass option on the BlockOptions SimulationOptions sheet for blocks within the optimization convergence loop. You can also specify this globally on the Setup SimulationOptions Calculations sheet.

4. Check to ensure that the manipulated variables affect the value of the objective function and/or the constraints, perhaps by performing a sensitivity analysis.
5. Provide a better starting estimate for the values of the manipulated variables.
6. Narrowing the bounds of the manipulated variables or loosening the tolerance on the objective function might help convergence.
7. Modify the parameters of the convergence block associated with the optimization (step size, number of iterations, etc.)

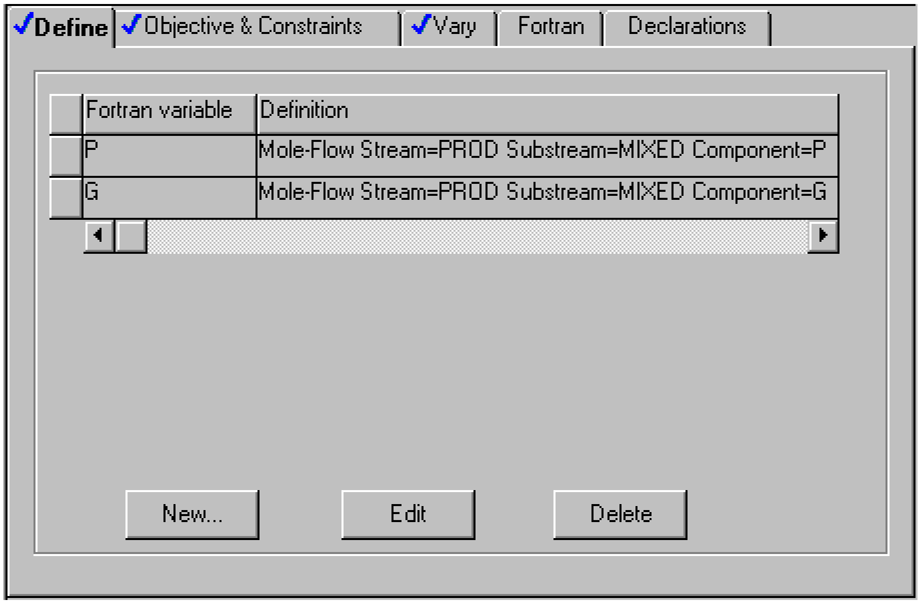
Example for Maximizing Product Value

The value of a reactor product stream is a function of the flow rate of the desired product, P, and the undesired byproduct, G.

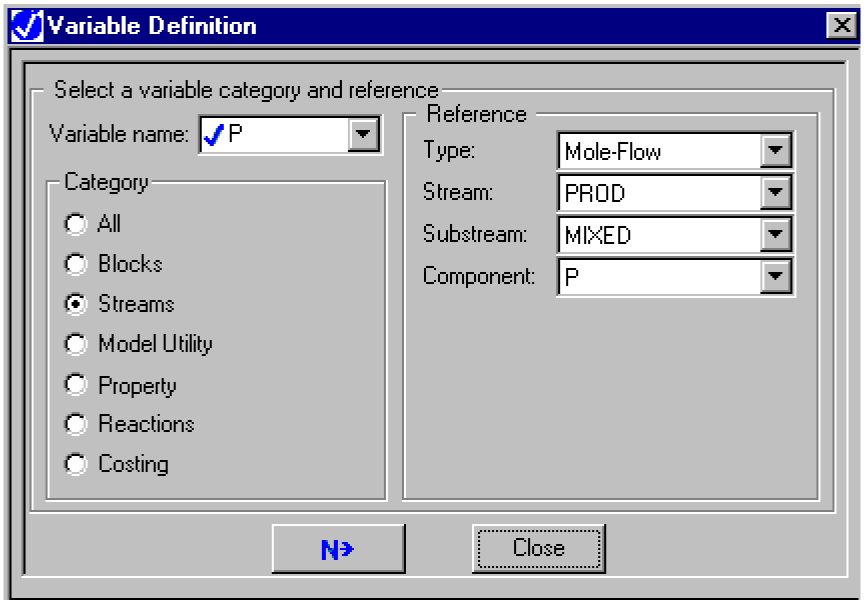
Value = P - 30 * G

Optimization is used to find the reaction temperature that maximizes the product value.

- The molar flow rate of components P and G in stream PROD are the sampled variables for the optimization. These variables are called P and G, respectively.
- The optimization objective function is (P - 30*G).
- You can use Fortran expressions, such as (P - 30*G) in any part of the optimization problem.
- The reactor temperature is the manipulated variable. The optimization convergence block finds the reactor temperature that makes (P - 30*G) a maximum.
- The manipulated variable is specified in the reactor block, just as if there were no optimization. The specified value is the initial estimate used by the optimization convergence block.
- The optimization convergence block will not try a temperature less than 300F or greater than 400F, even if the maximum of the objective function lies outside this range.
- You do not have to specify convergence of the optimization. Aspen Plus automatically generates a convergence block to converge the optimization.
- This optimization problem does not have any constraints associated with it.



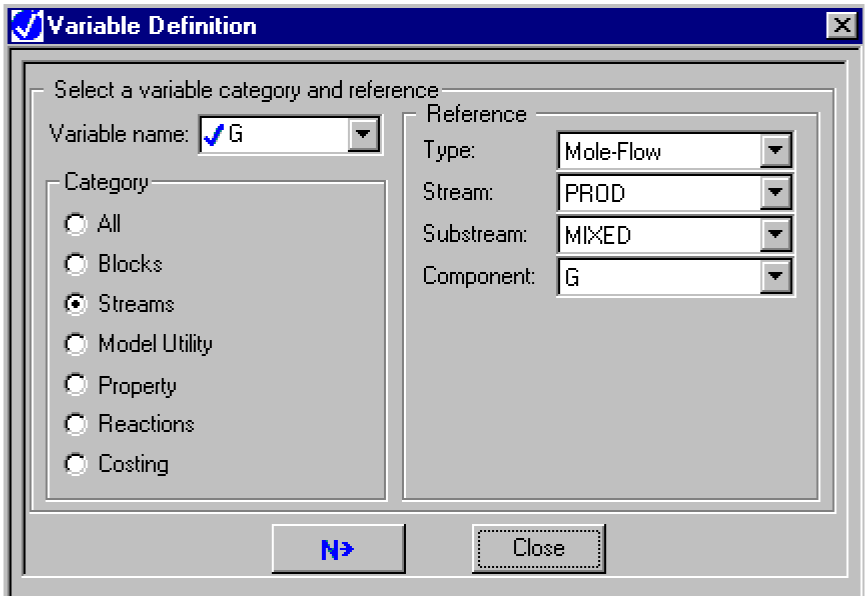
Fortran variable	Definition
P	Mole-Flow Stream=PROD Substream=MIXED Component=P
G	Mole-Flow Stream=PROD Substream=MIXED Component=G



Variable name: ✓P

○ All
○ Blocks
● Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

Type: Mole-Flow
Stream: PROD
Substream: MIXED
Component: P



Variable Definition

Select a variable category and reference

Variable name: G

Category
- ○ All
- ○ Blocks
- ● Streams
- ○ Model Utility
- ○ Property
- ○ Reactions
- ○ Costing

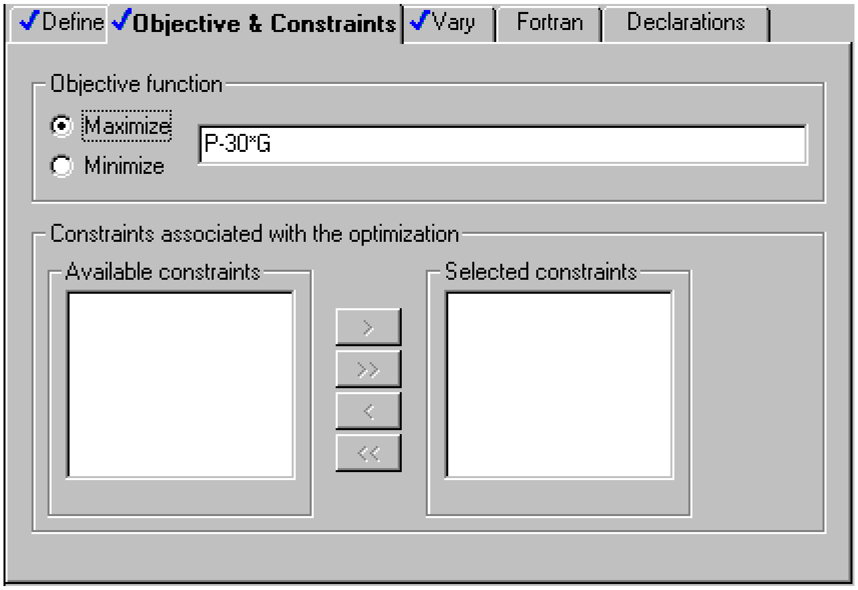
Reference

Type: Mole-Flow

Stream: PROD

Substream: MIXED

Component: G



Objective function

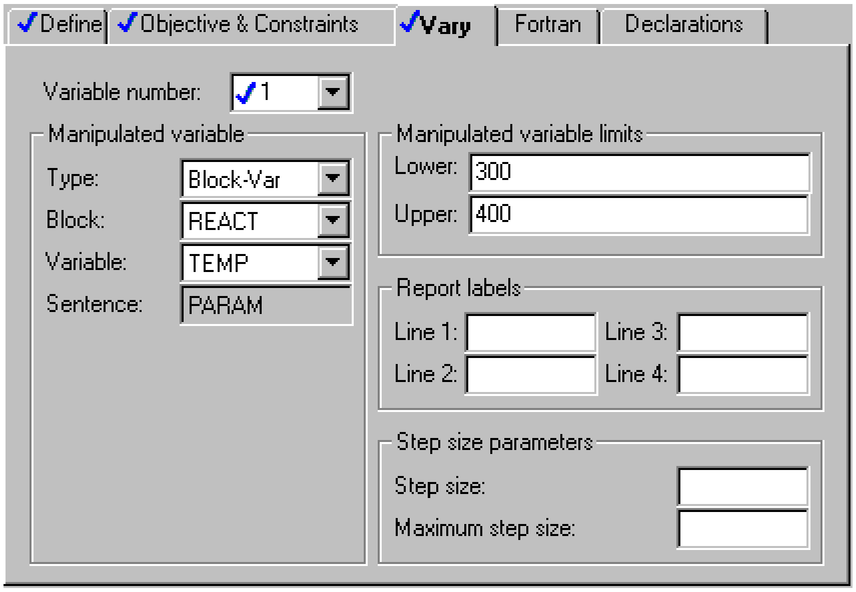
● Maximize
○ Minimize

P-30*G

Constraints associated with the optimization

Available constraints

Selected constraints



Variable number: ✓1

Type: Block-Var
Block: REACT
Variable: TEMP
Sentence: PARAM

Lower: 300
Upper: 400

Line 1:
Line 2:
Line 3:
Line 4:

Step size:
Maximum step size:

Example for Maximizing Operating Margin

The value of a process is calculated as the value of the product and the byproduct, minus the cost of the raw material, and minus the cost of steam for the reactor. The Fortran sheet is used to calculate the cost function:

```
C
C CPROD = PRICE OF PRODUCT, $/LB
         CPROD = 1.30
C
C CBYPR = PRICE OF BYPRODUCT, $/LB
         CBYPR = 0.11
C
C CFEED = PRICE OF FEED, $/LB
         CFEED = .20
C
C CSTEAM = COST OF STEAM, $/MMBTU
         CSTEAM = 4.00
C
C COST FUNCTION
         CFUNC = CPROD * P + CBYPR * G - CFEED * A - CSTEAM * Q /1D6
```

There are two constraints:

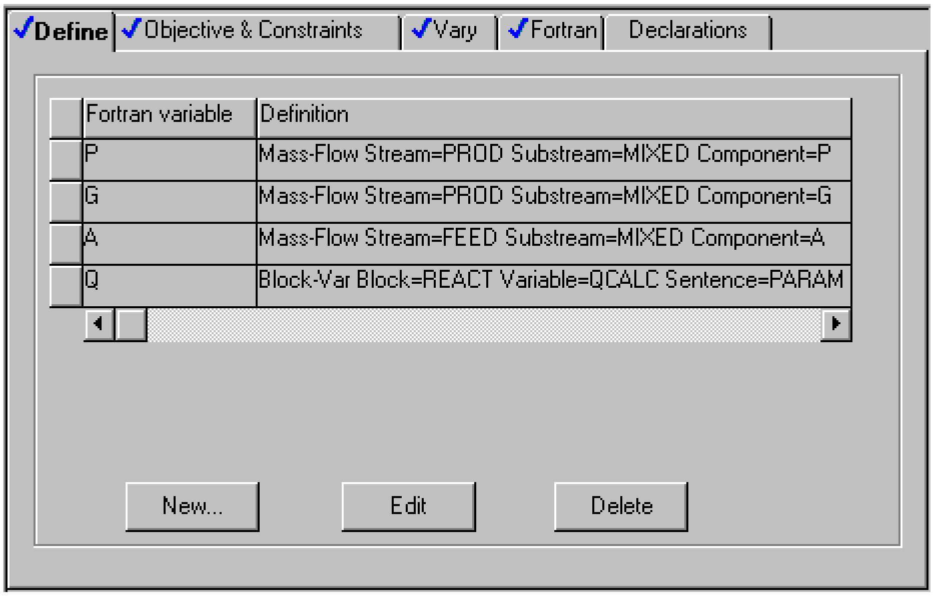
- Maximum duty for the reactor
- Minimum product purity.

Optimization is used to find the reaction temperature and the feed flow rate that maximizes the cost function.

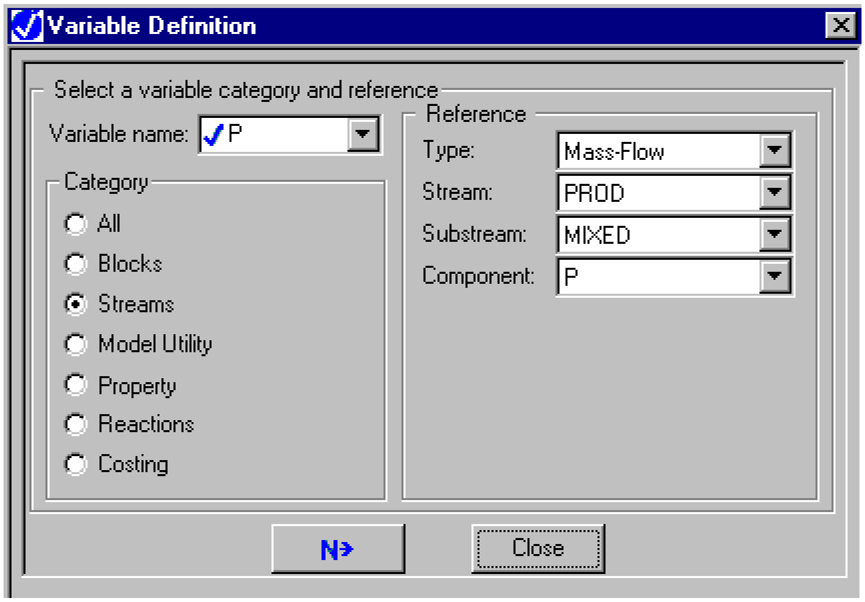
- The molar flow rate of P and of G in stream PROD, the molar flow rate of A in stream FEED and the reactor duty are the sampled variables for the optimization. These variables are called P, G, A, and Q, respectively.
- The optimization problem is converged when CFUNC is at a maximum.

- There are two manipulated variables: the reactor temperature and the flow rate for the reactant A in the feed. The optimization convergence block finds the combination of values that makes CFUNC a maximum subject to the constraints.
- The Fortran sheet is used to calculate the cost function CFUNC.
- The manipulated variables are specified in the blocks just as if there were no optimization. The specified value is the initial estimate used by the optimization convergence block.
- You do not have to specify convergence of the optimization. Aspen Plus automatically generates a convergence block to converge the optimization problem.
- There are two constraints associated with the optimization problem. They are called DUTY and PURITY.
- The constraint DUTY is satisfied when the reactor duty is less than or equal to 3 MMbtu/hr.
- The constraint PURITY is satisfied when mole fraction of P in the stream PROD is greater or equal to than 0.9.

On the Optimization sheets:



Fortran variable	Definition
P	Mass-Flow Stream=PROD Substream=MIXED Component=P
G	Mass-Flow Stream=PROD Substream=MIXED Component=G
A	Mass-Flow Stream=FEED Substream=MIXED Component=A
Q	Block-Var Block=REACT Variable=QCALC Sentence=PARAM



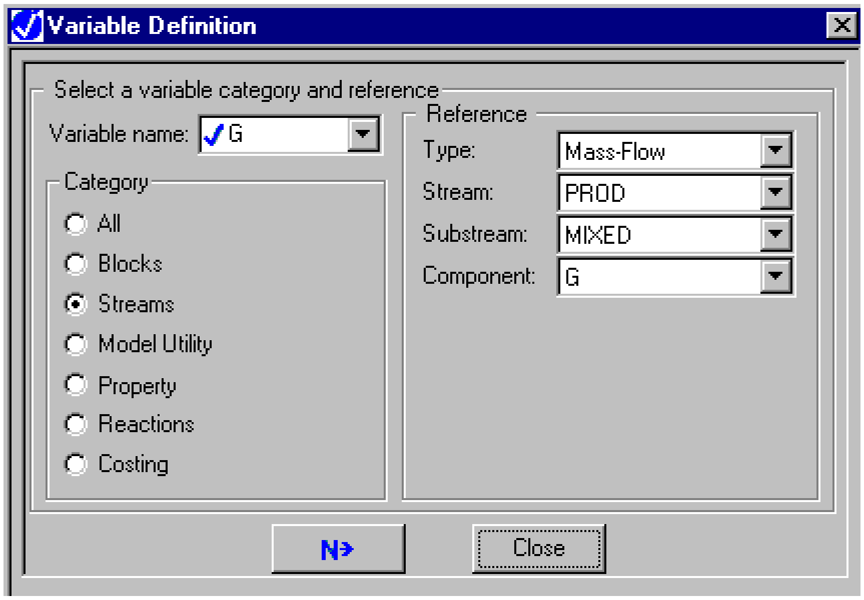
Variable Definition

Select a variable category and reference

Variable name: P

Category
○ All
○ Blocks
● Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

Reference
Type: Mass-Flow
Stream: PROD
Substream: MIXED
Component: P



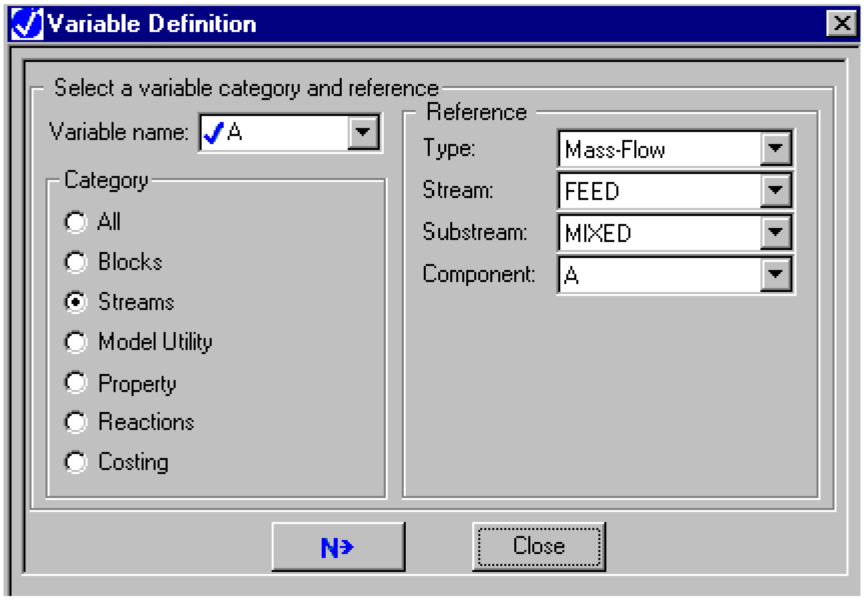
Variable Definition

Select a variable category and reference

Variable name: G

Category
○ All
○ Blocks
● Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

Reference
Type: Mass-Flow
Stream: PROD
Substream: MIXED
Component: G



Variable Definition

Select a variable category and reference

Variable name: A

Category
- ○ All
- ○ Blocks
- ● Streams
- ○ Model Utility
- ○ Property
- ○ Reactions
- ○ Costing

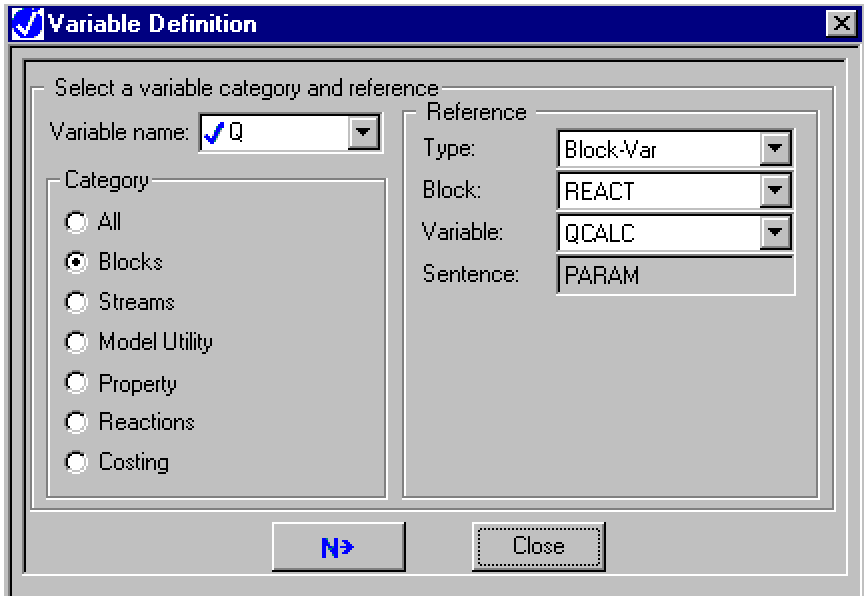
Reference

Type: Mass-Flow

Stream: FEED

Substream: MIXED

Component: A



Variable Definition

Select a variable category and reference

Variable name: Q

Category
- ○ All
- ● Blocks
- ○ Streams
- ○ Model Utility
- ○ Property
- ○ Reactions
- ○ Costing

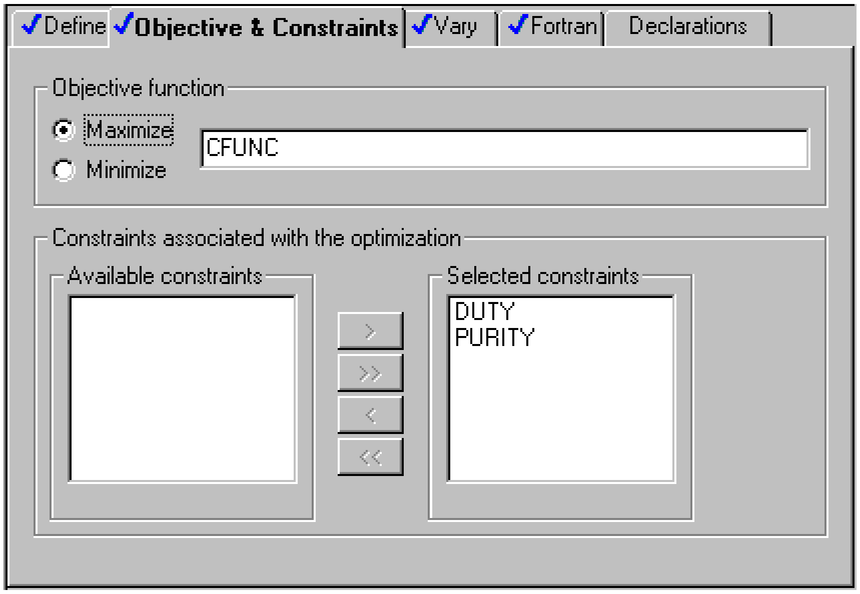
Reference

Type: Block-Var

Block: REACT

Variable: QCALC

Sentence: PARAM



Objective function

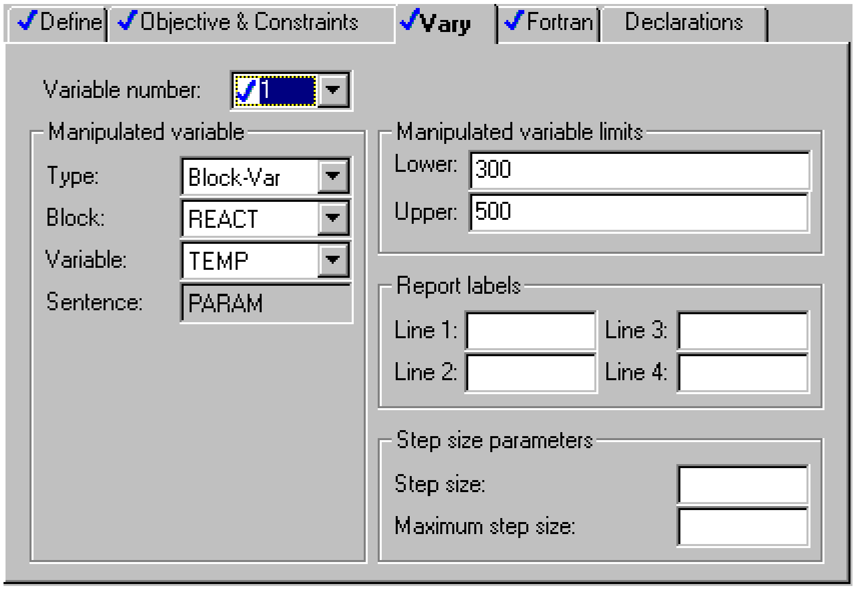
● Maximize: CFUNC

○ Minimize

Constraints associated with the optimization

Available constraints

Selected constraints:
DUTY
PURITY



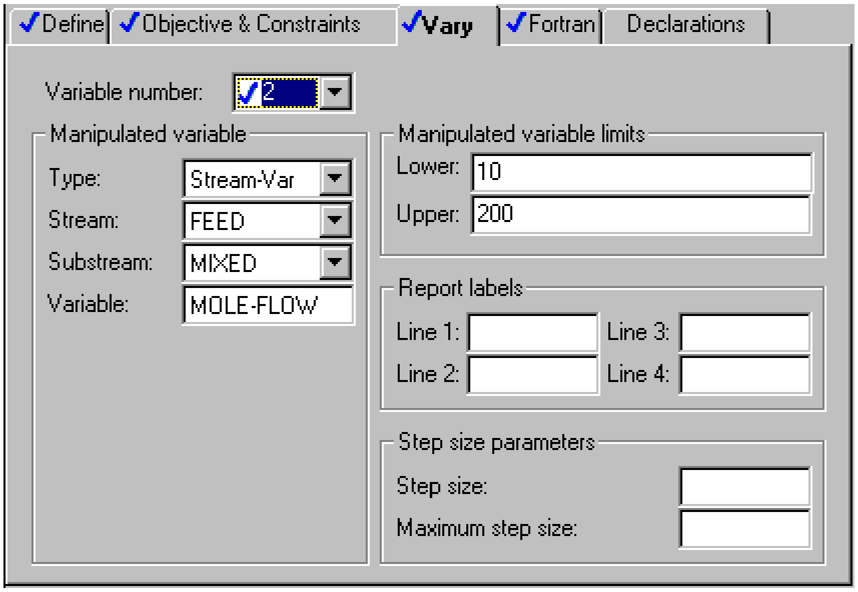
Variable number: ✓1

Manipulated variable
Type: Block-Var
Block: REACT
Variable: TEMP
Sentence: PARAM

Manipulated variable limits
Lower: 300
Upper: 500

Report labels
Line 1:
Line 2:
Line 3:
Line 4:

Step size parameters
Step size:
Maximum step size:



Variable number: 2

Type: Stream-Var

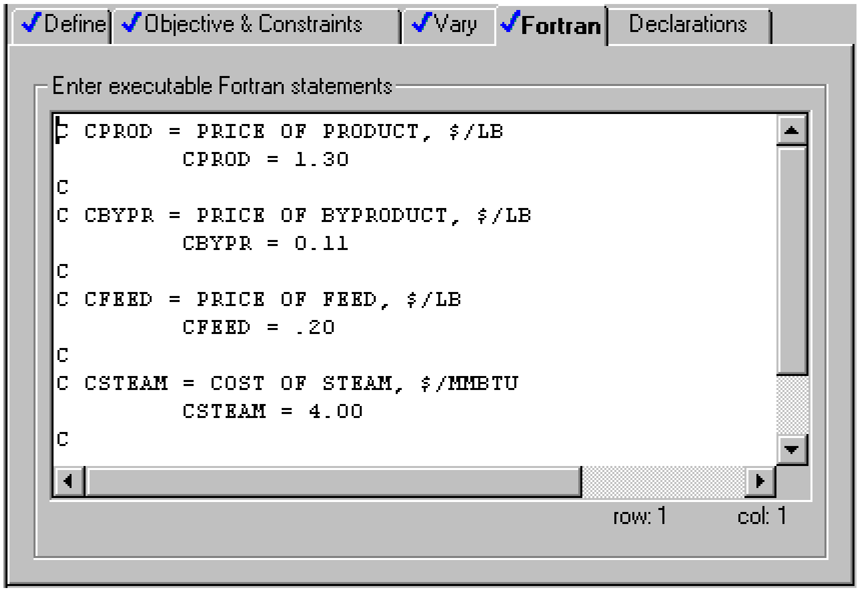
Stream: FEED

Substream: MIXED

Variable: MOLE-FLOW

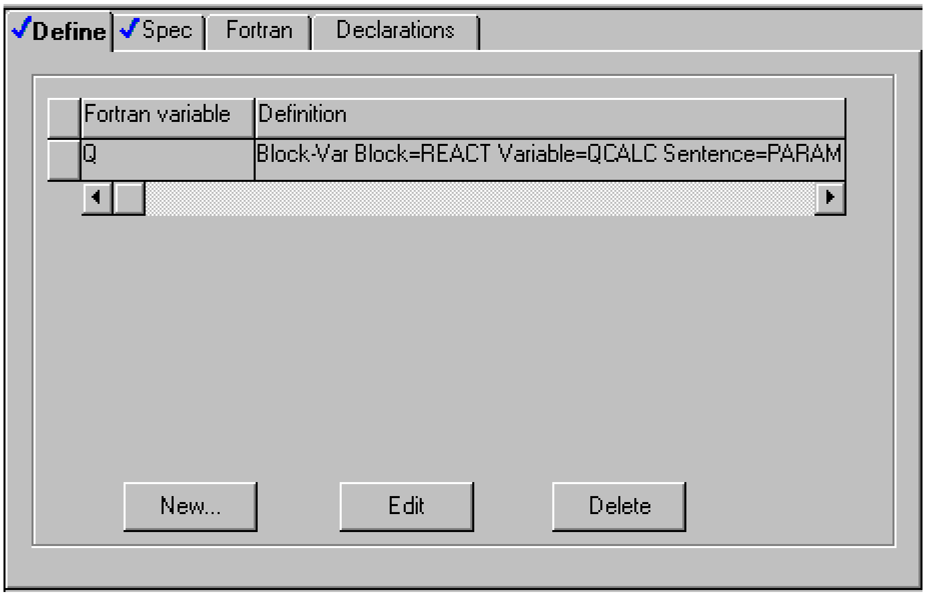
Lower: 10

Upper: 200

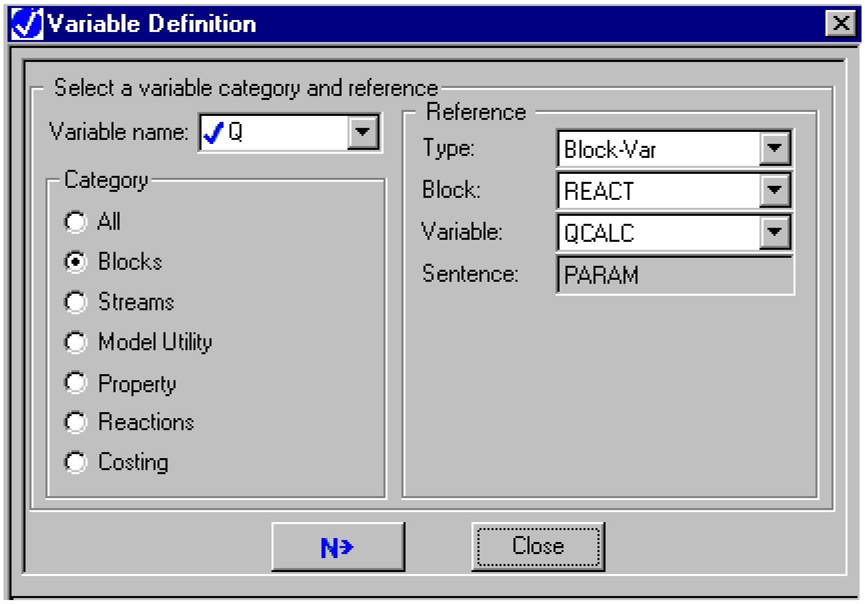


```
C CPROD = PRICE OF PRODUCT, $/LB
         CPROD = 1.30
C
C CBYPR = PRICE OF BYPRODUCT, $/LB
         CBYPR = 0.11
C
C CFEED = PRICE OF FEED, $/LB
         CFEED = .20
C
C CSTEAM = COST OF STEAM, $/MMBTU
         CSTEAM = 4.00
C
```

On the DUTY constraint sheets:



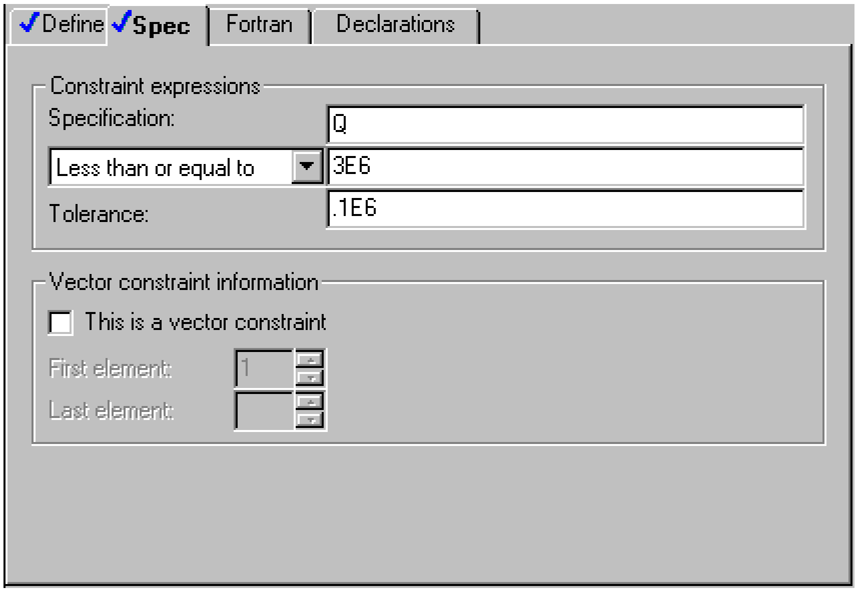
Fortran variable	Definition
Q	Block-Var Block=REACT Variable=QCALC Sentence=PARAM



Variable name: ✓Q

○ All
● Blocks
○ Streams
○ Model Utility
○ Property
○ Reactions
○ Costing

Type: Block-Var
Block: REACT
Variable: QCALC
Sentence: PARAM



Constraint expressions

Specification: Q

Less than or equal to 3E6

Tolerance: .1E6

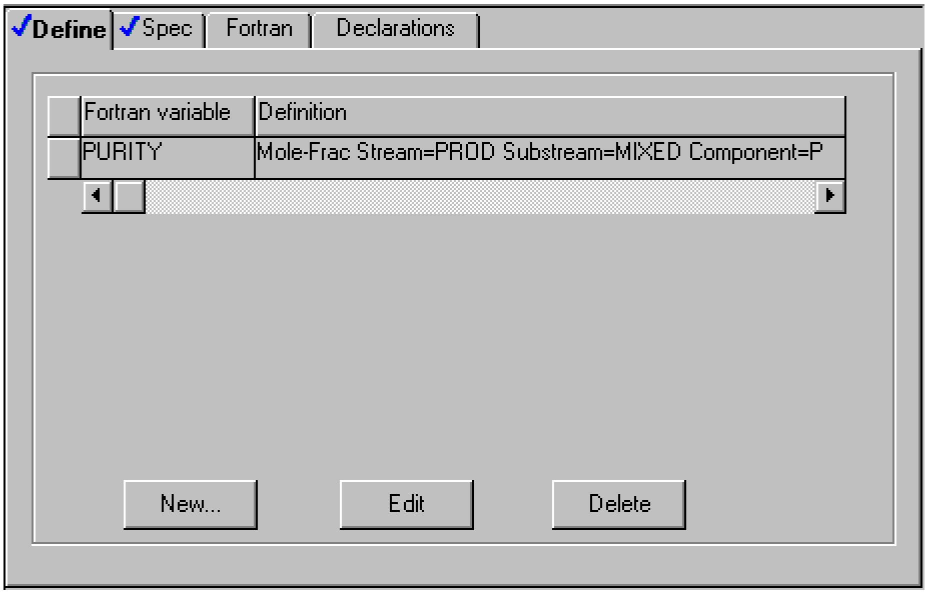
Vector constraint information

☐ This is a vector constraint

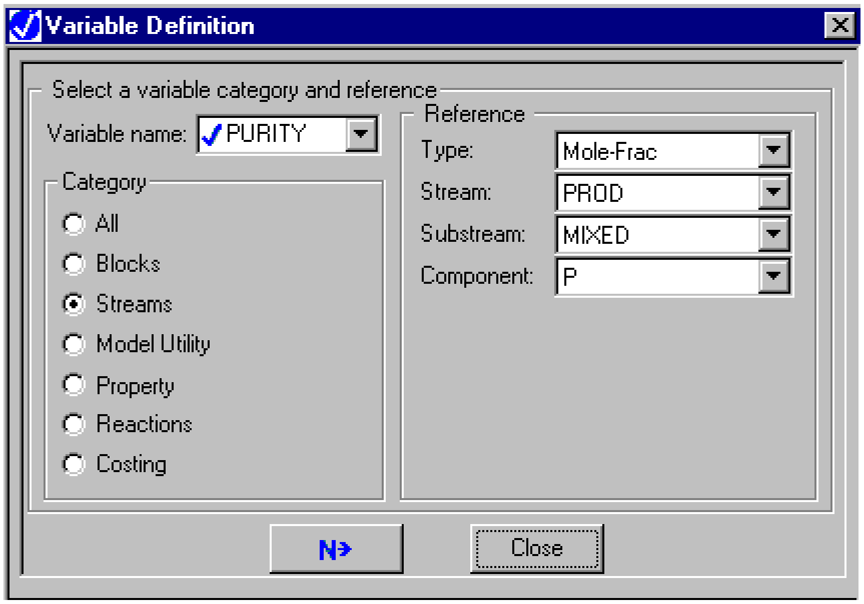
First element: 1

Last element:

On the PURITY constraint form:



Fortran variable	Definition
PURITY	Mole-Frac Stream=PROD Substream=MIXED Component=P



Variable name: PURITY

Category:
- ○ All
- ○ Blocks
- ● Streams
- ○ Model Utility
- ○ Property
- ○ Reactions
- ○ Costing

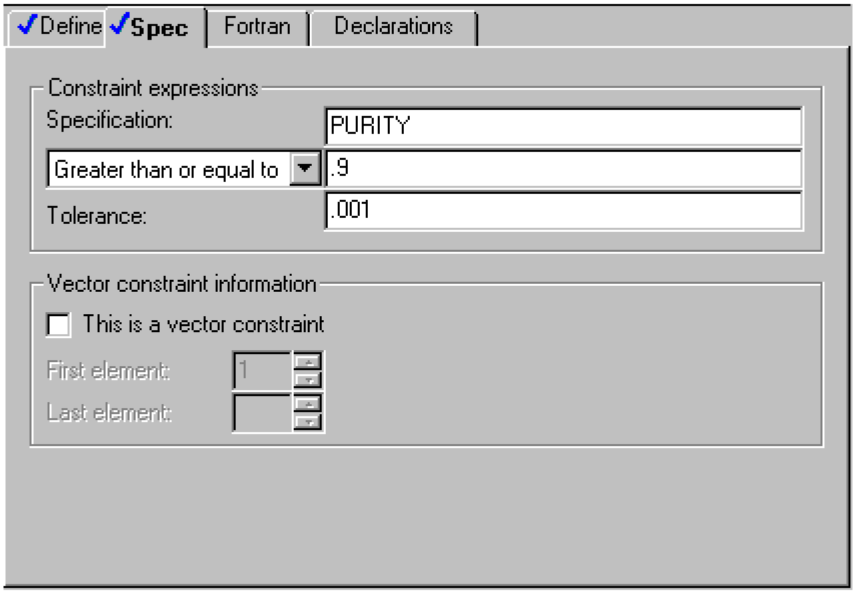
Reference:

Type: Mole-Frac

Stream: PROD

Substream: MIXED

Component: P



Specification: PURITY

Greater than or equal to .9

Tolerance: .001

☐ This is a vector constraint

First element: 1

Last element:

◆ ◆ ◆ ◆

23 Fitting a Simulation Model to Data

You can fit Aspen Plus simulation models to plant or laboratory data using Data-Fit. You provide one or more sets of measured data for input and results variables of a simulation model. Data-Fit adjusts (or estimates) input parameters to find the best fit of the model to the data. If you want Data-Fit to reconcile measured data for input variables to match the fitted model, it can do this simultaneously.

Data-Fit minimizes the weighted sum of squares of the differences between the measured data and the model prediction. In statistical terms, Data-Fit performs either ordinary least squares or maximum likelihood (errors-in-variables) estimation.

This chapter discusses:

- Types of Data-Fit applications
- Defining a Data-Fit problem
- Creating Point-Data sets
- Creating Profile-Data data sets
- Defining Data-Fit regression cases
- Ensuring well-formulated Data-Fit problems
- Analyzing convergence problems
- Examining results

Two comprehensive examples are given.

Types of Data-Fit Applications

Data-Fit applications fall into two main categories.

In the first type of application, Data-Fit determines coefficients for Aspen Plus user or built-in kinetics models from laboratory kinetics data. For example, given data for concentration versus time at one or more temperature, Data-Fit determines coefficients of the power law kinetics model.

In the second type of application, Data-Fit matches an Aspen Plus simulation to plant data as the first step in a simulation study. For example, given one or more sets of distillation column feed and product measurements, Data-Fit finds the column efficiency that best fits the measurements. At the same time, Data-Fit can:

- Adjust the measurements to match the fitted model
- Estimate missing feed or product measurements
- Help identify poor measurements

Data-Fit is designed for off-line use in developing an Aspen Plus simulation model that matches available data. Data-Fit is not designed for online plant data reconciliation applications.

Defining a Data-Fit Problem

Fitting a simulation model to data involves three major steps:

1. Creating base-case Aspen Plus model.

   For example, to fit concentration versus time kinetics data, create an RBatch model. The kinetics model coefficients you enter for RBatch using the Reactions forms become initial estimates for the Data-Fit problem.

2. Creating one or more Data-Fit data sets.

Use this Data Set type	To fit
POINT-DATA	• One or more steady-state experiments or operating points • Initial charge and final products of a batch reactor, but not intermediate time points • Feeds and products of a plug flow reactor, but not points along the length of the reactor
PROFILE-DATA	• Time series data for a batch reactor • Measurements along the length of a plug flow reactor

3. Defining regression cases. Specify Data-Fit cases and input parameters to be estimated. See Defining Data-Fit Regression Cases, this chapter.

Subsequent sections of this chapter describe each of these steps.

Creating Point-Data Data Sets

To create a Point-Data data set:

1. From the Data menu, point to Model Analysis Tools, then Data Fit.
2. On the left pane of the Data Browser, select Data-Set.
3. In the Data-Set Object Manager, click New.
4. In the Create New ID dialog box, enter an ID or accept the default ID.
5. In the Select Type list, select Point-Data and click on OK.
6. On the Define sheet, identify the flowsheet variables for which you have measurements (see Identifying Flowsheet Variables, this chapter).
7. On the Data sheet, enter the measured data (see Entering the Measured Point-Data, this chapter).

Identifying Flowsheet Variables

You must identify the flowsheet variables for which you have measurements. Use the Data-Fit Data-Set Define sheet to identify the flowsheet variables used in the data set and assign them variable names. The variable name identifies the flowsheet variable on other data set sheets.

Use the Define sheet to identify a flowsheet variable and assign it a variable name. When completing a Define sheet, specify the variables on the Variable Definition dialog box. The Define sheet shows a concise summary of all the accessed variables, but you cannot modify the variables on the Define sheet.

On the Define sheet:

1. To create a new variable, click the New button.

   or

   To edit an existing variable, select a variable and click the Edit button.
2. Type the name of the variable in the Variable Name field. If you are editing an existing variable and want to change the variable name, click the right mouse button on the Variable Name field. On the popup menu, click Rename. A variable name must:
   - Be six characters or less for a scalar variable
   - Be five characters or less for a vector variable
   - Start with an alphabetic character (A – Z)
   - Have subsequent alphanumeric characters (A – Z, 0 – 9)
   - Not begin with IZ or ZZ

3. In the Category frame, use the option button to select the variable category.
4. In the Reference frame, select the variable type from the list in the Type field.

   Aspen Plus displays the other fields necessary to complete the variable definition.
5. Click Close to return to the Define sheet.

See Chapter 18, Accessing Flowsheet Variables for more information on accessing variables.

Tip Use the Delete button to quickly delete a variable and all of the fields used to define it.

Tip Use the Edit button to modify the definition of a variable in the Variable Definition dialog box.

Types of Flowsheet Variables

You must identify the flowsheet variables for which you have measurements. You can also identify results variables for which you have no measurements. Aspen Plus will estimate the results variables and tabulate them for each data point.

In Data-Fit, you cannot access vectors. You must access each stream variable or each component in a composition vector as a different scalar variable.

Always access feed stream compositions as mole, mass, or standard volume component flows. Do not access them as fractions. This avoids any problems with normalizing fractions.

You can access both input values and results values for certain flowsheet variables. For example, the condenser duty of a RadFrac block can be accessed either as the input variable Q1 or the results variable COND-DUTY. The reboiler duty can be accessed as the input variable QN or as the results variable REB-DUTY. Select either the input or results variable as follows:

Is the measured variable specified as an input in the base case simulation?	Then select
Yes	The input variable
No	The results variable

For example, suppose:

- Your base-case model consists of a RadFrac block with Reflux Ratio and Condenser Duty specified.
- The data you want to fit includes reboiler and condenser duty.

You must select the results variable REB-DUTY for the reboiler duty, since it is not specified as an input in the base-case model. You must select the input variable Q1 for the condenser duty, since it is specified as an input in the base-case model.

If you want to reconcile the measurement for Q1, provide a non-zero standard deviation. If you do not want to reconcile it, provide a zero standard deviation.

Entering the Measured Point-Data

Use the Data-Fit Data-Set Data sheet to enter measured data.

For each measured variable:

1. On the Data-Fit Data-Set form, click the Data tab.
2. Specify whether the variable is a simulation Input or Result for the Data-Fit problem.

Specify these variables	As
Measured feed stream	Input
Measured product stream	Result
Measured variables that were accessed as input variables on the Define sheet	Input
All other measured variables	Result

Note Intermediate stream variables are usually results. However, when a Data-Fit problem spans only a subset of the flowsheet, you must specify intermediate streams that are inlets to the Data-Fit subproblem as inputs.

3. Specify a standard deviation for the measurement in the first row of the data table.
4. Enter one or more data points (rows in the table). If a measurement is not available for a Result variable, leave its Data field blank. Data-Fit will estimate it. You must always enter a value for an Input variable.

You can introduce a new standard deviation row at any time. It will apply to subsequent data points.

Standard Deviation

The standard deviation is the level of uncertainty in the measurement. You can enter it as an absolute or percent error (append a percent sign (%) to the value). Statistically determined standard deviations are seldom available. It is enough to supply an approximate “expected error,” estimated from experiences or instrument specifications. Each residual (measurement — model prediction) term in the sum of squares function is weighted by 1/(standard deviation^2).

You must specify a standard deviation greater than zero for each results variable to be fit. If a zero value is entered for standard deviation, that results variable is not included in the regression.

For inputs, a standard deviation greater than zero invokes maximum likelihood (errors-in-variables) estimation:

If the standard deviation for an input variable is	Then Aspen Plus
Zero	Treats the measurement as exact and Data-Fit does not adjust it
Greater than zero	Adjusts (reconciles) the measurement, along with results measurements, to match the fitted model **Note** Reconciling inputs can increase solution time significantly, since each reconciled input is treated as a decision variable by the least squares algorithm

Creating Profile-Data Sets

To create a Profile-Data data set:

1. On the Data menu, select Model Analysis Tools, then Data Fit.
2. On the left pane of the Data Browser, select Data-Set
3. In the Data-Set Object Manager, click New.
4. In the Create New ID dialog box, enter an ID or accept the default ID.
5. In the Select Type list, select Profile-Data and click on OK.
6. On the Define sheet, identify the flowsheet variables for which you have measurements (see Identifying Profile Variables, this chapter).
7. On the Data sheet, enter the measured data (see Entering the Measured Profile-Data, this chapter).
8. You can specify the charge (Rbatch) or feed (Rplug) on the Initial Conditions sheet.

Identifying Profile Variables

Profile variables are available for the RBatch and RPlug unit operation models.

1. On the Data-Set form, click the Define tab.
2. In the Model and Block Name area, select either RBatch or the RPlug.
3. In the Block field, identify the block where the profiles have been measured.
4. In the Variable Name field, enter a variable name. A variable name must:
   - Be six characters or less for a scalar variable
   - Start with an alphabetic character (A – Z)
   - Have subsequent alphanumeric characters (A – Z, 0 – 9)
   - Not begin with IZ or ZZ
5. In the Variable list, select a variable. See the prompt for a description of each variable.
6. For concentration or fraction profile variables, identify the component being measured in the Component field. You must identify each component concentration or fraction as a separate measured variable.
7. Repeat steps 4 through 6 for each measured variable.

You can identify profile variables for which you have no measurements. Data-Fit will calculate and tabulate them.

Entering the Measured Profile-Data

Use the Data-Fit Data-Set Data sheet to enter measured data.

For each measured variable:

1. On the Data-Fit Data-Set form, click the Data tab.
2. In the first row of the data table, specify a standard deviation greater than zero for each measured variable to be fit. If a zero value is entered for the standard deviation, that results variable is not included in the regression.
3. Enter the time or length and the measurements for each data point. Leave missing measurements blank. Aspen Plus will estimate them.

   You can introduce a new standard deviation row at any time. It will apply to subsequent data points.
4. If you want to specify temperature and pressure values to replace those in the base-case, enter the value(s) on the Initial Conditions sheet. Data-Fit does not reconcile (adjust) these values. It assumes they are exact.

5. If the experiment was carried out with a feed or charge different than that in the base-case model, specify the component flows on the Profile-Data Initial Conditions sheet. Select the basis (Mole/Mass/StdVol) and the units. Enter the component flows. Aspen Plus assumes the values you enter are exact and does not adjust them. You can only specify flows for conventional components. If the feed/charge specified in the base-case model contains nonconventional components, Data-Fit will use:
   - Base-case specifications for nonconventional components
   - Conventional component flows entered on this form as feed/charge to reactor

The standard deviation is the level of uncertainty in the measurement. See Standard Deviation, this chapter, for more information.

Defining Data-Fit Regression Cases

You can fit both Point-Data and Profile-Data data sets in the same regression case. For example, you might have time series data for a reaction at one temperature (Profile-Data), and overall conversion data at several temperatures (Point-Data).

A Data-Fit regression case must involve at least one of the following:

- An estimated parameter
- A reconciled input (with a standard deviation greater than zero)

Aspen Plus adjusts (reconciles) measured input variables when you specify non-zero standard deviations for the input measurements on the Data-Set Data sheet. There will be one estimate for a reconciled measured input for each data point.

For an estimated parameter, you must have already entered a value for it as an input specification for the base simulation, or it must have a default value. Data-Fit uses this specification as the initial guess for the variable.

If the base-case value lies outside the bounds you enter for the parameter on the Regression Vary sheet or for a reconciled input, Data-Fit uses the nearest bound as the initial guess.

There is no limit to the number of estimated parameters.

Data-Fit leaves a variable at its lower or upper limit if violating the limit would further decrease the sum-of squares function.

Creating Data-Fit Regression Cases

To define a Data-Fit regression case:

1. On the Data menu, select Model Analysis Tools, then Data Fit.
2. On the left pane of the Data Browser, select Regression.
3. In the Regression Object Manager, click New.
4. In the Create New ID dialog box, enter an ID or accept the default ID.
5. On the Specifications sheet, identify the data sets to be fit in the case (see Creating Point-Data Data Sets and Creating Profile-Data Sets, this chapter). You can also supply Weights to adjust the relative weighting of the data sets, but this is usually not necessary. For more information on Weights see Data-Fit Numerical Formulation.
6. On the Vary sheet, identify any simulation input parameters you want to estimate. Data-Fit will adjust the variables to find the best fit to the Data-Sets listed on the Specifications sheet.
7. On the Convergence sheet, you can select the Initialization Method when reconciling input measurements.

To initialize the reconciled inputs to	Use the initialization method
Base-case values	Base Ccase Values (default)
Measured values	Measurements

The default base-case initialization method is robust, but it can take a few more iterations if the measurements are far off from the base case.

Normally you do not need to change any other defaults on the Regression Convergence sheet. See Convergence Parameters, this chapter, for more information.

Convergence Parameters

The Regression Convergence sheet is used to specify optional Data-Fit convergence parameters. In most cases, it is unnecessary to change these parameters from their default values.

The following parameters are available on the Convergence sheet:

Field	Default	Used To
Maximum Algorithm Iterations	50	Specify the maximum number of optimizer iterations.
Maximum Passes Through Flowsheet	1000	Set the maximum number of flowsheet passes allowed in a Data-Fit run. Included in the count of flowsheet passes are the initial base case, passes required to compute the residuals, and passes required to compute the Jacobian matrix through perturbation.
Bound Factor	10	Lower and Upper bounds for reconciled input variables are computed using Bound Factor times Standard Deviation for that variable. See Bound Factor, this chapter, for more information about setting the Bound Factor.
Absolute Function Tolerance	0.01	Specify the absolute sum-of-squares objective function tolerance. If the optimizer finds a point where the objective function value is less than the Absolute Function Tolerance, the problem is converged.
Relative Function Tolerance	0.002	Specify the relative function convergence tolerance. If the current model predicts a maximum possible function reduction of at most the relative function tolerance times the absolute value of the function value at the start of the current iteration, and if the last step attempted achieved no more than twice the predicted function decrease, then the problem is considered converged.
X Convergence Tolerance	0.002	Specify the X convergence tolerance. If a step is tried that has a relative change in X less than or equal to the X Convergence Tolerance and if this step decreases the objective function by no more than twice the predicted objective function decrease, the problem is considered converged.
Minimum Step Tolerance	1e-10	Data-Fit returns with suboptimal solution if a step of scaled length of at most Minimum Step Tolerance is tried but not accepted.
Calculate Covariance Matrix	checked	Calculate covariance and correlation matrices and write correlation matrix to report file.

Advanced Parameters

The Regression Advanced sheet is used to specify additional Data-Fit convergence parameters. In most cases, it is unnecessary to change these parameters from their default values.

The algorithm maintains an estimate of the diameter of a region about the current estimate of the vector of varied values in which it can predict the behavior of the least-squares objective function, that is, a trust region.

The following parameters are available on the Convergence sheet:

Trust region tuning parameters field	Default	Used To
Switching Parameter	1.5	Data-Fit algorithm uses a trust-region strategy. Switching Parameter is used in a test to decide when to switch the model for the trust region.
Adjustment Factor	0.75	If the decrease in the value of the objective function is at least Adjustment Factor*inner product of the step and the gradient, then the trust region radius is increased.
Reduction Factor	0.5	The factor by which the trust region radius is shrunk if current X leads to errors in function or Jacobian evaluation.
Minimum Reduction Factor	0.1	The minimum factor by which the trust region radius may be shrunk.
Minimum Expansion Factor	2	The minimum factor by which the trust region radius is increased if it is increased at all.
Maximum Expansion Factor	4	The maximum factor by which the trust region radius may be increased at one time.

Step and tuning parameters field	Default	To
Initial Step Size	1	Factor determining the initial step size of the trust region. The choice of Initial Step Size can profoundly affect the performance of the algorithm - different values sometimes lead to finding different local minima. Too small or too large a value of Initial Step Size causes the algorithm to spend several function evaluations in the first iteration increasing or decreasing the size of the trust region.
Size Control Parameter	0.0001	For the step to be accepted the actual function reduction must be more than Size Control Parameter times its predicted value.
Adaptive Scaling Strategy	0.6	Tuning factor associated with adaptive scaling strategy in the algorithm
Relative Perturbation Size	0.005	Default perturbation size during Jacobian evaluation for variable X is Relative Perturbation Size times the absolute value of X.
False Convergence Check Parameter	0.1	Helps decide when to check for false convergence and to consider switching the algorithm model for the current trust region.

Data-Fit Numerical Formulation

Data-Fit solves a problem with the following formulation:

$$\underset{Xp,\,Xri}{Min}\frac{1}{2}\sum_{i=1}^{Nsets}\left(W_i*\left(\sum_{j=1}^{N\exp i}(term1+term2)\right)\right)$$

$$term1=\sum_{l=1}^{Nri}\left((Xmri-Xri)/\sigma_{Xmri}\right)^2$$

$$term2=\sum_{m=1}^{Nrr}\left((Xmrr-Xrr)/\sigma_{Xmrr}\right)^2$$

subject to $Xp_{lb} \le Xp \le Xp_{ub}$

$Xri_{lb} \le Xri \le Xri_{ub}$

Where:

Nsets = Number of data sets specified on the Regression Specifications sheet

Nexpi = Number of experiments in data set i

Nri = Number of reconciled input variables

Nrr = Number of measure results variables

Wi = Weight for data set I specified on the Regression Specifications sheet

Xp = Vector or varied parameters

Xmri = Measured values of the reconciled input variables

Xri = Calculated values of the reconciled input variables

Xmrr = Measured values of the results variables

Xrr = Calculated values of the results variables

Sigma = Standard deviation specified for the measured variables

Reconciled input variables are adjusted to minimize the sum of square of errors for each experiment independently.

Ensuring Well-Formulated Data-Fit Problems

This section applies primarily to Point-Data data sets.

Although Data-Fit is extremely flexible, you must ensure that a Data-Fit problem is well posed. Data-Fit does not check this for you. There are two basic rules you must follow:

- When Data-Fit evaluates a data point, it merges the current values of the measured inputs and the estimated parameters with the base-case specifications. To avoid erroneous results, the set of measured inputs for a data set must form a complete input specification for uniquely calculating the measured results for that data set.
- The base-case simulation model must be formulated to have a solution, even when the measurements are not in mass or energy balance.

The following example illustrates the application of both rules.

Example of a Well-Formulated Data-Fit Problem

Suppose you want to fit column efficiency to operating data for a distillation column with one feed and two products. Data are available for several operating points. Each operating point has:

- A different feed composition, flow rate, and temperature
- Different distillate and bottoms flow rates and temperatures
- The same reflux ratio and feed and column pressures

The feed data consists of component mole flow rates and temperatures. Product stream data consists only of total flow rates and temperatures.

The following table describes a well-posed Data-Fit formulation for this problem:

This	Consists of
The base-case simulation model	• A feed stream with temperature, pressure, and component mole flows specified • A RadFrac block with Mole Reflux Ratio, Mole Distillate to Feed Ratio, and pressure specified
The data set for the operating points	Inputs: • Mole flow rate for each component with a non-zero flow in the base-case feed stream • Feed stream temperature • Distillate-to-feed ratio, accessed as the RadFrac Mole-D:F input variable and entered as an unmeasured input in the data set Results: • Distillate and bottoms temperature • Distillate and bottoms flow rate

The pressure and Mole Reflux Ratio are fixed specifications for this problem. Data-Fit overrides the base-case feed component flow rates, temperature, and column distillate-to-feed ratio specification for the evaluation of each data point. If any inputs were omitted from the data set, base-case values would be used for the data point evaluations, causing incorrect results.

The distillate-to-feed ratio specification must be used so that RadFrac can solve with most any feed. If the distillate flow specification were used instead, a measure distillate rate that was not in good mass balance with the measured feeds could result in an infeasible column specification that RadFrac could not solve.

Bound Factor

When you specify non-zero standard deviations for measured inputs, Data-Fit uses the following limits for the variable estimates:

*Lower Bound = Measured value - (Bound Factor) * (Standard Deviation)*

*Upper Bound = Measured value + (Bound Factor) * (Standard Deviation)*

Bound Factor has a default value of 10. You can enter a different value on the Regression Convergence sheet.

Aspen Plus checks to see whether the lower bound for flows is negative. If so, a warning is given and the lower bound is set to zero. Care should be taken in setting the Bound Factor to avoid zero flow rates.

Remember that setting bounds that are too tight or too loose could cause Data-Fit to move into an infeasible region. For example, if you are reconciling the reflux rate for a tower and using the reflux rate as a reconciled input variable, and you allow the lower bound on the reflux rate to be zero, Data-Fit may drive the reflux rate to zero during the solution process and cause severe errors in RadFrac.

Instead of setting very tight bounds on the reconciled input variables, you should treat them as fixed instead.

Estimating Unmeasured Variables

Data-Fit can estimate and tabulate any unmeasured result. Access the calculated variable as a Result in a data set, enter a nonzero standard deviation, and leave the data field blank.

Data-Fit can also estimate unmeasured input variables. Access the variable as an Input in a data set. Enter a reasonable initial guess and a large standard deviation (for example, 50%) for the variable. Make sure the standard deviation gives reasonable lower and upper limits for the estimated variable.

Sequencing Data-Fit

For Data-Fit problems, Aspen Plus will:

1. Run the base-case simulation.
2. Execute the Data-Fit loop until it converges or fails to converge.
3. Replace the base-case values of fitted parameters with the regressed values, and rerun the base-case simulation.

If any Case-Study or Sensitivity blocks are present, Aspen Plus uses the fitted parameters to generate the Case-Study and/or Sensitivity tables. The Data-Fit problem is not re-executed each time.

The Aspen Plus automatic sequencing algorithm places Data-Fit loops outside any flowsheet convergence loops.

In most cases, Data-Fit should be run standalone. For example, you may want to estimate kinetic coefficients in the power-law expression, using a RCSTR block. Run Data-Fit with RCSTR. Then use the regressed values as input in a larger flowsheet with that RCSTR block.

You can sequence the execution manually to suit your needs on the Convergence Sequence form.

Using Data-Fit Results

The key Data-Fit results are:

Results	On Data-Fit sheet
Chi-Square statistic for the fit	Regression Results Summary
Final estimates and standard deviations for the estimated parameters	Regression Results Manipulated Variables
Table of measured values, estimated values, and normalized residuals for the data sets	Regression Results Fitted-Data
Table of iteration history of the function results or of the vary results and reconciled input	Regression Results Iteration History

A Chi-Square value greater than the threshold value indicates the model does not fit the data. This can occur due to errors in the measured data, or because the model does not represent the data. You can use the Chi-Square statistic for selecting between models. If you fit two or more models to the same data set(s), the model with the lowest Chi-Square value fits the data best.

It is not uncommon for the standard deviations of estimated parameters to be relatively large. This does not necessarily indicate a poor fit.

Review the Regression Results Fitted-Data sheet for large normalized residuals (outliers). A residual value much larger than the others might indicate a bad data point.

For measured inputs with standard deviations equal to zero, there are no estimated values or residuals. Data-Fit does not adjust these measurements.

The Regression Results Fitted-Data sheet allows the plotting of results. These plots can help you:

- Visualize how well your model fits the data
- Spot poor data points

For information about how to generate plots, see Chapter 13 .

Troubleshooting

If Data-Fit fails to converge, look for:

- Large errors in the values entered for the measurements, such as data entry errors or incorrect units
- Gross errors in source data

Errors may occur in the problem formulation. Check:

- Does the base-case simulation converge?
- Do measured inputs completely determine the measured results? See Ensuring Well-Formulated Data-Fit Problems, this chapter.
- Is the base-case simulation formulated to handle measured data that are not in good mass balance? See Ensuring Well-Formulated Data-Fit Problems, this chapter.
- Do the values specified in the base-case simulation provide good estimates for the estimated parameters?
- Do the estimated parameters affect the measured variables over the range specified? You can check the sensitivity of the measured variables to the estimated parameters with a sensitivity run. A different base-case parameter value or a smaller parameter range may be needed.

- Do specified bounds allow the decision variables to take the model into infeasible regions (leading to convergence failures for unit operation model algorithms or internal convergence loops)? The recommended action is to tighten the bounds.
- Do the fitted parameters have large differences in order of magnitude? If so, it may be helpful to scale those values using a Fortran block.
- Does the model represent the data? If not, either choose another model or enter new base-case specifications.

Example of Fitting Reaction Kinetics Data

Determine the coefficients of the Aspen Plus power law kinetics model for the liquid phase reaction ALLYL + ACET → PROD. A backup file for this problem is included in the Examples library as datafit1.bkp.

The following data is available:

Initial charge:	0.05 lb ALLYL
	0.07 lb ACET
Reaction temperature:	30°C

Mole fractions:

Time	ALLYL	PROD
600 seconds	0.30149	0.19745
900 seconds	0.25613	Unmeasured
1900 seconds	0.14938	0.45820

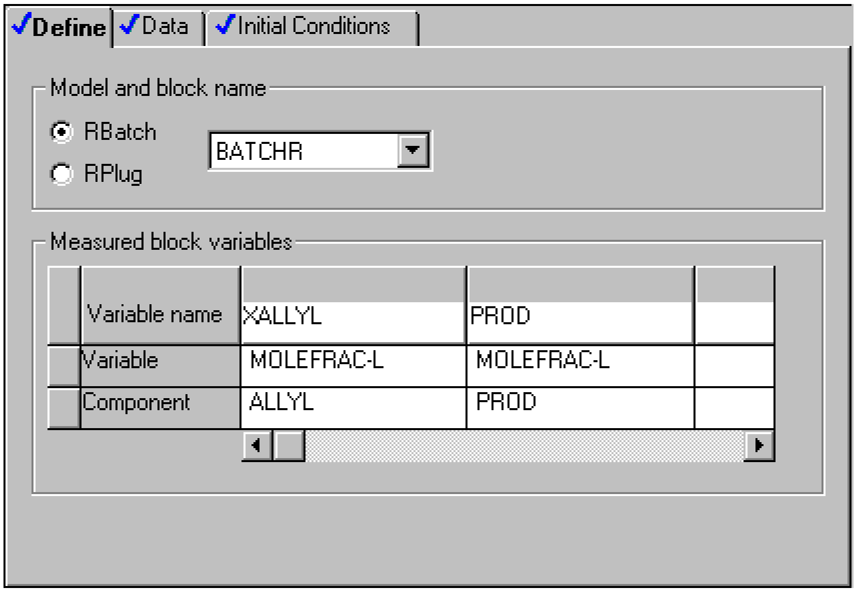
A base-case simulation is defined with the following specifications:

Feed	Flow Rate
ALLYL	0.05 lb/hr
ACET	0.07 lb/hr

Rbatch Specification	Value
Reactor Type	Constant Temperature
Temperature	30.0°C
Cycle time	1900.0 seconds
Valid phases	Liquid-Only

Power Law Kinetics Specifications	Value
ALLYL exponent	1.0
ACET exponent	0.5
Pre-exponential factor	1.5E7
Activation energy	6.5E7

Time series data is entered in a Profile-Data data set.



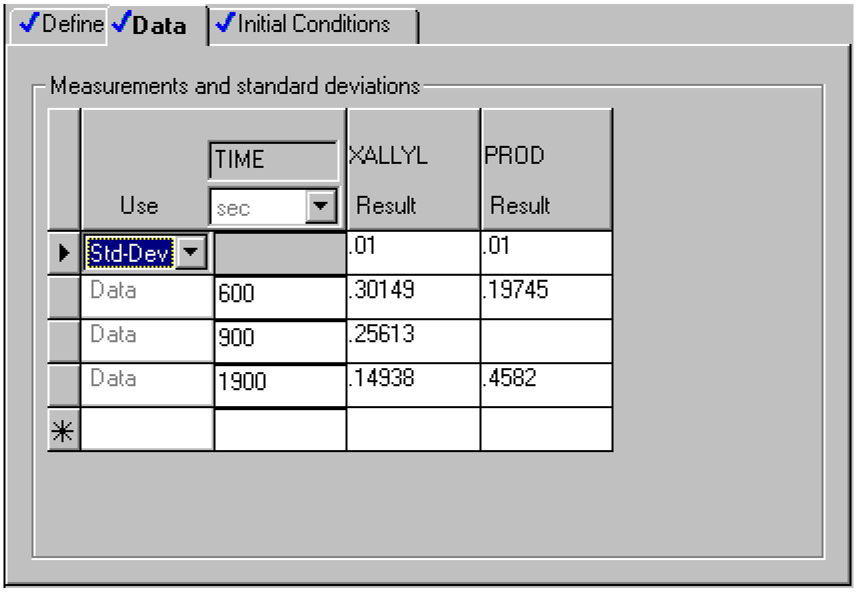
Model and block name

● RBatch
○ RPlug

BATCHR

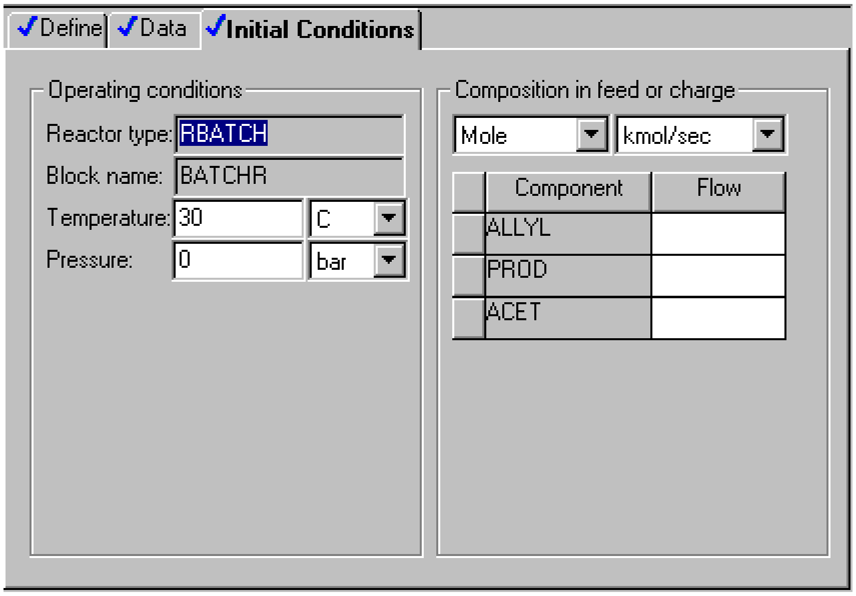
Measured block variables

Variable name	XALLYL	PROD
Variable	MOLEFRAC-L	MOLEFRAC-L
Component	ALLYL	PROD



Measurements and standard deviations

Use	TIME sec	XALLYL Result	PROD Result
Std-Dev		.01	.01
Data	600	.30149	.19745
Data	900	.25613	
Data	1900	.14938	.4582



Operating conditions

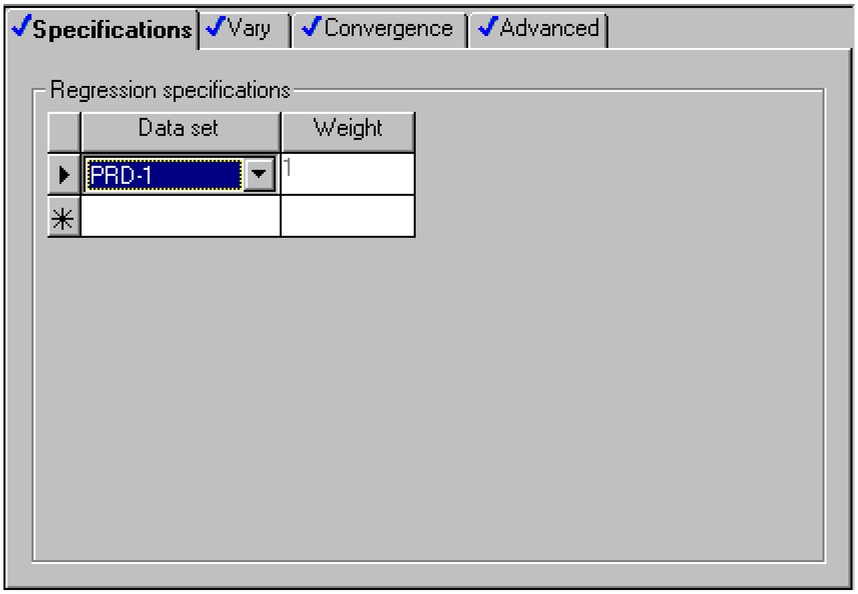
Reactor type: RBATCH
Block name: BATCHR
Temperature: 30 C
Pressure: 0 bar

Composition in feed or charge

Mole
kmol/sec

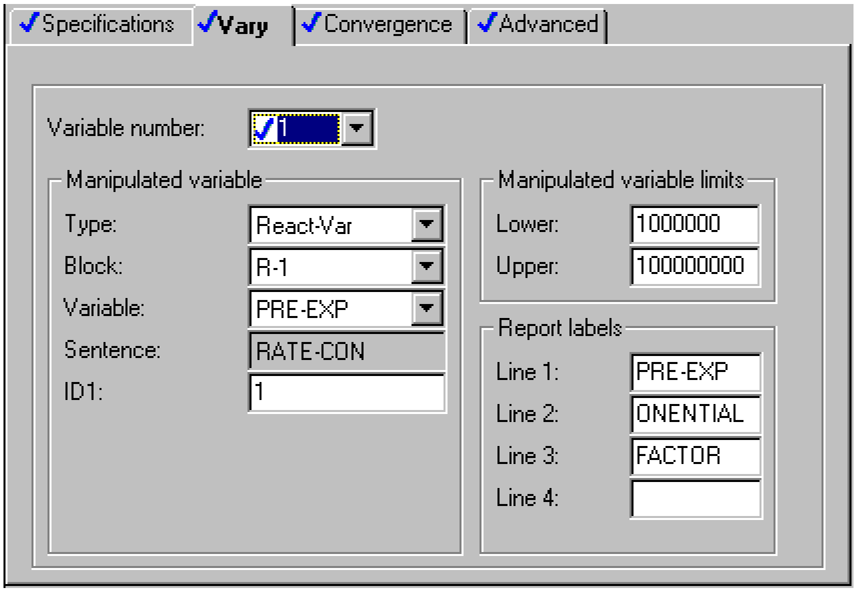
Component	Flow
ALLYL	
PROD	
ACET	

Because data is available at only one temperature, the pre-exponential factor is fit with the activation energy fixed. The Regression case is entered as follows:



Regression specifications

Data set	Weight
PRD-1	1



Variable number: ✓1

Manipulated variable

Type: React-Var

Block: R-1

Variable: PRE-EXP

Sentence: RATE-CON

ID1: 1

Manipulated variable limits

Lower: 1000000

Upper: 100000000

Report labels

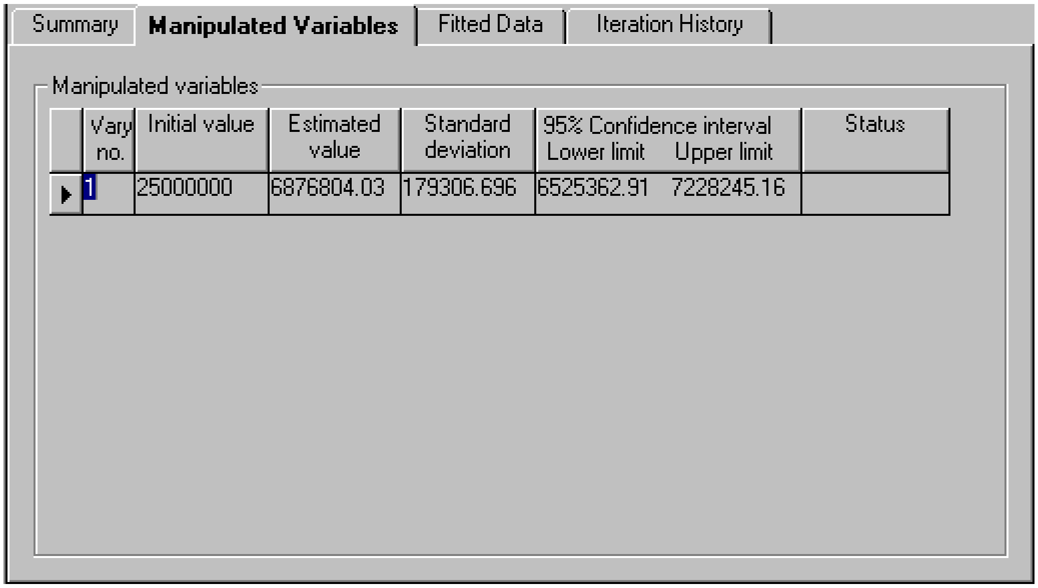
Line 1: PRE-EXP

Line 2: ONENTIAL

Line 3: FACTOR

Line 4:

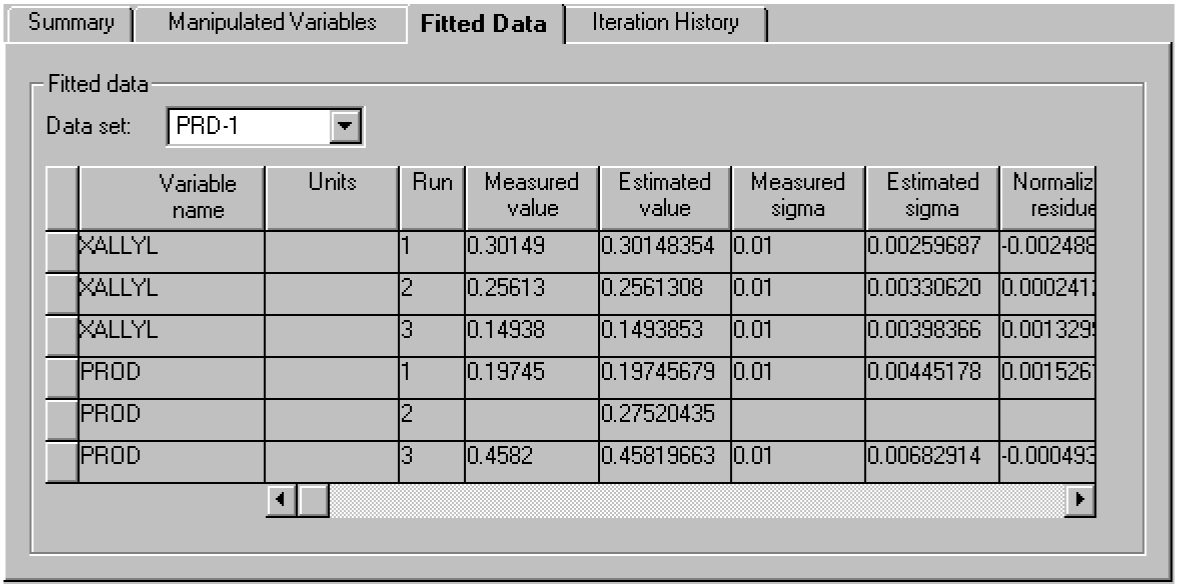
After running the Data-Fit problem, the resulting estimate of the pre-exponential factor appears on the Regression Results Manipulated Variable sheet:



Manipulated variables

Vary no.	Initial value	Estimated value	Standard deviation	95% Confidence interval Lower limit	Upper limit	Status
1	25000000	6876804.03	179306.696	6525362.91	7228245.16	

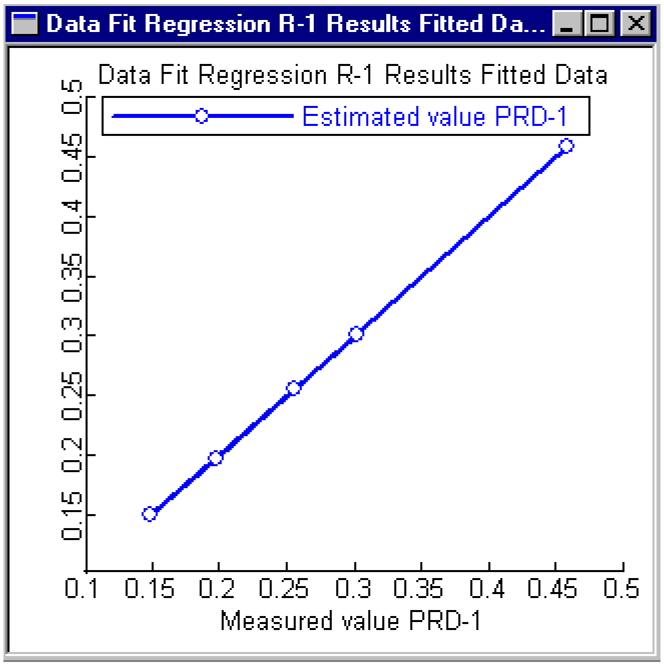
The Regression Results Fitted-Data sheet displays the original measured values, along with the final estimated values for these variables.



Data set: PRD-1

	Variable name	Units	Run	Measured value	Estimated value	Measured sigma	Estimated sigma	Normaliz residue
	XALLYL		1	0.30149	0.30148354	0.01	0.00259687	-0.002488
	XALLYL		2	0.25613	0.2561308	0.01	0.00330620	0.000241
	XALLYL		3	0.14938	0.1493853	0.01	0.00398366	0.001329
	PROD		1	0.19745	0.19745679	0.01	0.00445178	0.001526
	PROD		2		0.27520435			
	PROD		3	0.4582	0.45819663	0.01	0.00682914	-0.000493

These original measured values and the final estimated values can be plotted against each other to see the fit of the data and identify any outliers.



Example for Matching a Column Model to Plant Data

This example reconciles measurements and fits column Murphree stage efficiency to operating data for a binary distillation column with one feed and two product streams. A backup file for this problem is in the Examples library as datafit2.bkp.

The following data is available:

	Run 1	Run 2	Run 3
Feed			
Water flow rate, lbmol/hr	55	45	50
Ethanol flow rate, lbmol/hr	45	55	50
Temperature, °F	77	75	80
Distillate			
Total flow rate, lbmol/hr	45	55	50
Temperature, °F	175	170	174
Bottoms			
Total flow rate, lbmol/hr	45	55	50
Temperature, °F	180	185	183

A base-case simulation is defined with the following specifications:

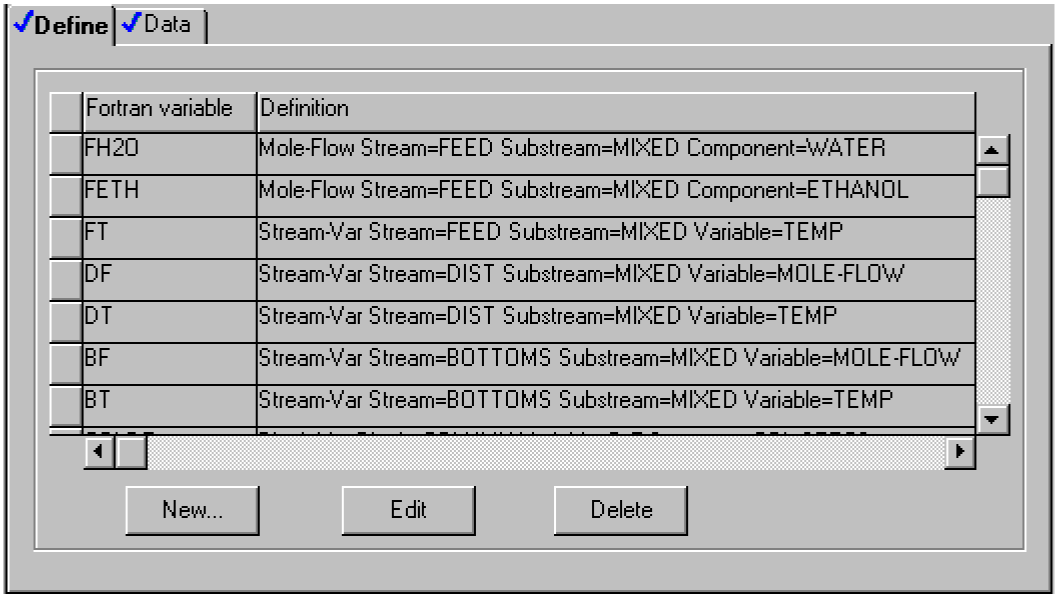
Feed Stream Specification	Value
Water flow rate, lbmol/hr	50
Ethanol flow rate, lbmol/hr	50
Temperature, °F	77
Pressure, psia	15

RadFrac Specification	Value
Number of stages	20
Feed stage	10
Pressure, psia	15
Distillate vapor fraction	0.0
Reflux ratio	3.0
Distillate-to-feed ratio	0.5
Murphree stage efficiencies	0.1

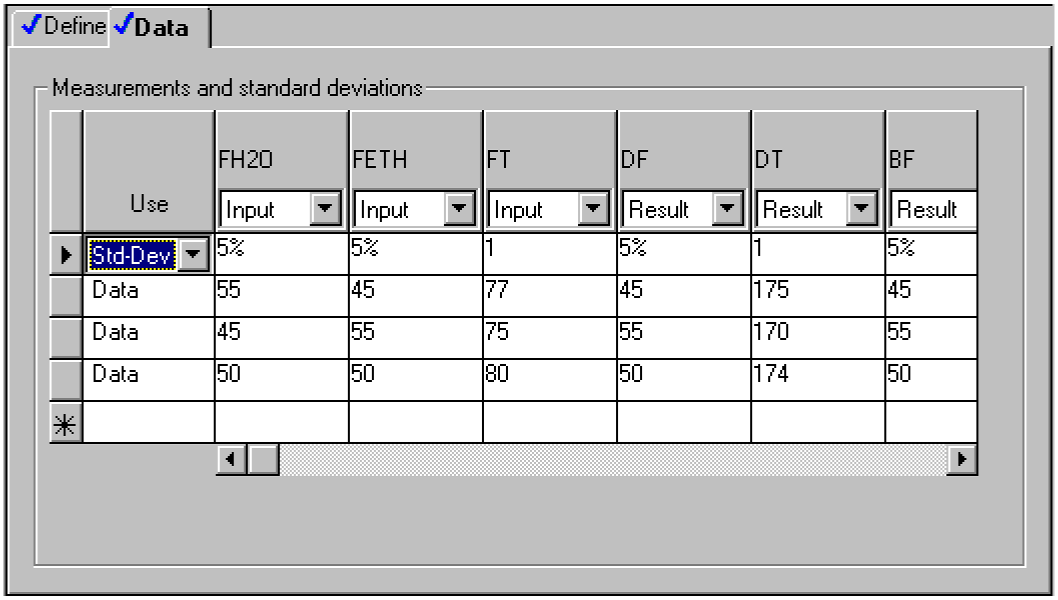
The column specifications (reflux ratio and distillate-to-feed ratio) ensure that the column can be solved even if the measured feed and distillate flow rates are not in mass balance.

A Fortran block is defined to set the stage efficiency of the column and is executed just before the RadFrac block. This Fortran block reads a parameter being varied by Data-Fit and transfers this to the efficiency of the first and last stages of the column. RadFrac automatically uses this efficiency for all intermediate stages.

The Point-Data data set is:



Fortran variable	Definition
FH2O	Mole-Flow Stream=FEED Substream=MIXED Component=WATER
FETH	Mole-Flow Stream=FEED Substream=MIXED Component=ETHANOL
FT	Stream-Var Stream=FEED Substream=MIXED Variable=TEMP
DF	Stream-Var Stream=DIST Substream=MIXED Variable=MOLE-FLOW
DT	Stream-Var Stream=DIST Substream=MIXED Variable=TEMP
BF	Stream-Var Stream=BOTTOMS Substream=MIXED Variable=MOLE-FLOW
BT	Stream-Var Stream=BOTTOMS Substream=MIXED Variable=TEMP



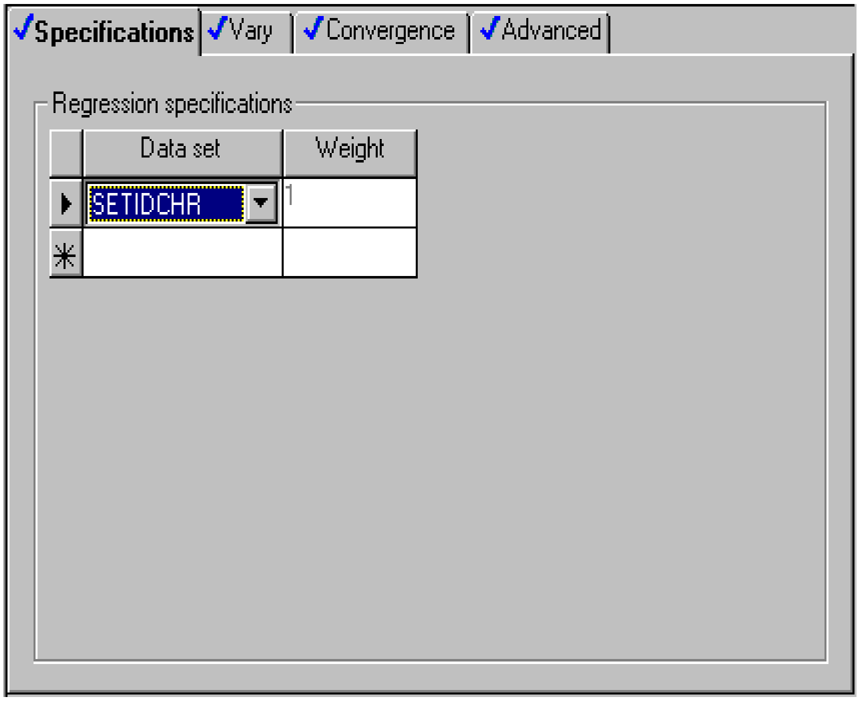
Measurements and standard deviations

Use	FH2O	FETH	FT	DF	DT	BF
	Input	Input	Input	Result	Result	Result
Std-Dev	5%	5%	1	5%	1	5%
Data	55	45	77	45	175	45
Data	45	55	75	55	170	55
Data	50	50	80	50	174	50

The distillate-to-feed ratio (COLDF) measurement is given an arbitrary value (0.5) and a large standard deviation (100.0). This specification tells Data-Fit to vary the distillate-to-feed ratio as needed for each data point to find the best fit to the measured data. The initial guess is 0.5. The distillate-to-feed ratio is an unmeasured input, to be estimated. Distillate and bottoms flow rate are treated as measured results. This ensures a feasible solution for the column for each Data-Fit data point.

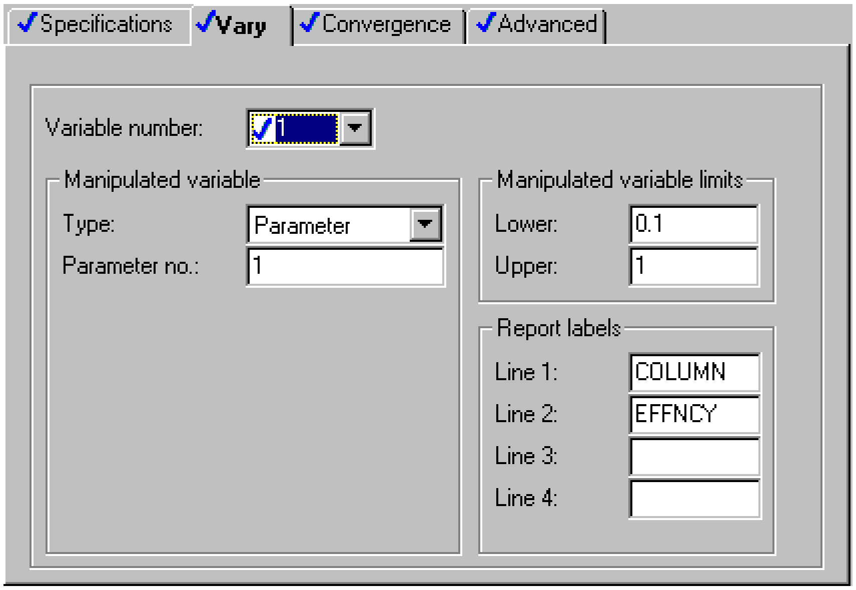
The measured distillate or bottoms flow rate could have been used directly as an input (the RadFrac specification). But, RadFrac would be unable to find a solution if the flow rate measurements contained significant error and were not in mass balance.

The Data-Fit Regression case is defined as follows:



Regression specifications

Data set	Weight
SETIDCHR	1



Variable number: ✓1

Type: Parameter

Parameter no.: 1

Lower: 0.1

Upper: 1

Line 1: COLUMN

Line 2: EFFNCY

Line 3:

Line 4:

❖ ❖ ❖ ❖

24 Transferring Information Between Streams or Blocks

Use a transfer block to copy the values of flowsheet variables from one part of the flowsheet to another. You can copy to any number of destinations:

- Whole streams
- Stream composition and flow rate
- Any flowsheet variable (for example, block variables)

The most common application is to copy one stream into another.

This chapter describes:

- Defining transfer blocks
- Creating transfer blocks
- Copying streams
- Copying flowsheet variables
- Specifying when to execute a transfer block
- Entering flash specifications for destination streams

Defining a Transfer Block

To define a transfer block:

1. Create the transfer block.
2. Copy either a stream, a stream flow, a substream or a block or stream variable.
3. Optionally enter flash specifications for destination streams.

By default, Aspen Plus will flash modified streams automatically, using the values present in the stream and the flash options established either on the Streams form for process feeds, or by the source block for other streams.

4. Optionally specify when the transfer block is executed.

   By default, Aspen Plus will sequence the block automatically.

Subsequent sections of this chapter describe each of these steps.

Creating a Transfer Block

To create a transfer block:

1. From the Data menu, point to Flowsheeting Options, then click Transfer.
2. In the Transfer Object Manager, click New.
3. In the Create New ID dialog box, enter an ID, or accept the default, and click OK.

Copying Flowsheet Variables

The From and To sheets are used to specify what flowsheet variables are copied from one place to another.

The following information can be copied:

If you select on the From sheet	Aspen Plus copies
Entire stream	An entire stream
Stream flow	Only the component flows and total flow of a stream
Substream	An entire substream
Block or stream variable	A scalar stream variable or block variable When scalar variables are copied, the variable type does not have to be the same on each sheet, but each variable type must have the same physical dimensions (for example temperature).

Copying Streams

To copy a stream:

1. On the Transfer form, click the From tab.
2. Click the Entire Stream option and specify the stream in the Stream Name field. The information for an entire stream including all substreams will be copied.
3. Click the To tab.
4. Specify any number of destination streams in the Stream field.

Copying Stream Flow

To copy component flows of a stream:

1. On the Transfer form, click the From tab.
2. Click the Stream Flow option and specify the stream in the Stream Name field. The component and total flow rates of a stream will be copied, but not the conditions (temperature, pressure, vapor fraction, and other intensive variables).
3. Click the To tab.
4. Specify any number of destination streams in the Stream fields.

Copying Substreams

To copy a substream:

1. On the Transfer form, click the From tab.
2. Click the Substream option and specify the stream and substream in the Stream Name and Substream fields. The information for one substream of a stream will be copied.
3. Click the To tab.
4. Specify any number of destination streams in the Stream and Substream fields.

Copying Block or Stream Variables

To copy a block, stream, or other flowsheet variable:

1. On the Transfer form, click the From tab.
2. Select the Block or Stream Variable option.
3. In the Type field, select the type of variable you want to copy.
4. Aspen Plus takes you to the remaining fields necessary to completely identify the variable. See Chapter 18 for more information on accessing variables.
5. Click the To tab.
6. On the Variable Number field, click the down arrow and select <new>.
7. In the Type field, select the type of variable for the destination of the copy.
8. Aspen Plus takes you to the remaining fields necessary to completely identify the variable.

   Repeat steps 6 to 8 for all the variables to which the From variable is to be copied.

Specifying Transfer Block Execution

Use the Transfer Sequence sheet to specify when the transfer block is executed.

You can do either of the following:

- Use the default, Automatically Sequenced, to let Aspen Plus sequence the block automatically.
- Specify when the Transfer block is to be executed (Before or After a block, or at the beginning (First) or end (Last) of a simulation).

To specify transfer block execution:

1. On the Transfer form, click the Sequence tab.
2. This table shows how to specify when the transfer block is to be executed:

Specify this in the Execute field	To
Automatically sequenced	Have the Transfer block sequenced automatically
First	Have the Transfer block executed at the beginning of the simulation
Before	Have the Transfer block executed before a specified Block, Convergence, Fortran, Transfer, Balance, or Pressure Relief The Block Type and Block Name must be specified.
After	Have the Transfer block executed after a specified Block, Convergence, Fortran, Transfer, Balance, or Pressure Relief The Block Type and Block Name must be specified.
Last	Have the Transfer block executed at the end of the simulation

3. If you entered Before or After, select the unit operation block, convergence block, Fortran block, transfer block, balance block or pressure relief black before or after which you want the transfer block to be executed.
4. Use the Diagnostics button on this sheet to set the levels of diagnostic output.

Entering Flash Specifications for Destination Streams

When you copy into a stream, Aspen Plus flashes the destination stream(s) to calculate a new set of stream properties using the values present in the stream and the flash options established either on the Streams form for process feeds, or by the source block for other streams.

You can use the optional Stream Flash sheet to specify the thermodynamic condition and flash options for modified streams. For example, use it when you copy stream flows and need to specify the temperature and pressure of the destination stream.

The flash type must be specified. The possible flash types are:

- Temperature & Pressure
- Temperature & Vapor Fraction
- Temperature & Enthalpy
- Pressure & Vapor Fraction
- Pressure & Enthalpy
- Do not Flash Stream

Temperature or pressure estimates can be entered if desired.

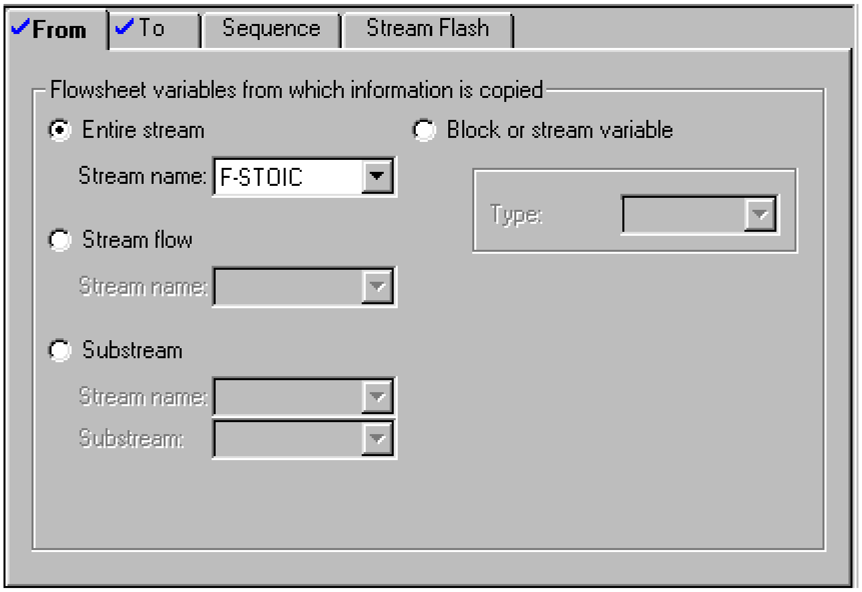
Also specify the phases the flash calculation should consider and optionally the maximum iterations and error tolerance for the flash calculation.

To enter flash specifications for a stream:

1. On the Transfer form, click the Stream Flash tab.
2. Specify the stream name in the Stream field.
3. Specify the Flash Type.
4. Specify the flash specifications, estimates and/or convergence parameters.

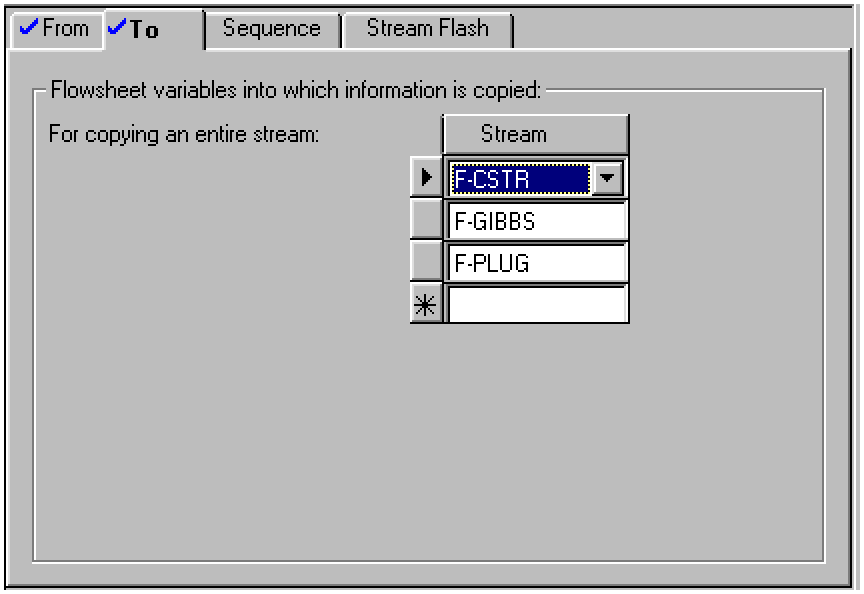
Example of a Stream Copied to Two Other Streams

A transfer block is used to copy stream F-STOIC into streams F-CSTR, F-PLUG, and F-GIBBS.



● Entire stream

Stream name: F-STOIC



Flowsheet variables into which information is copied:

For copying an entire stream:

Stream
F-CSTR
F-GIBBS
F-PLUG

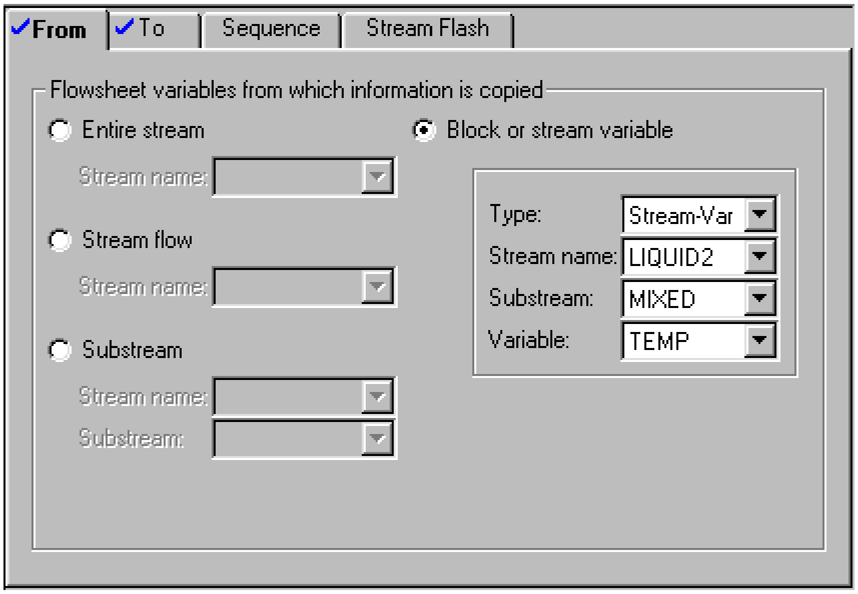
Example of Stream Conditions Copied to a Block

The transfer block TEMP sets the temperature of block TRANSFER equal to the temperature in stream LIQUID2.

The stream LIQUID2 is an outlet from a Flash3 where the properties are being calculated using the UNIF-LL physical property methods. Downstream from the Flash3, the properties are being calculated using the NRTL physical property methods.

When two different physical property methods are being used in a flowsheet, there may be inconsistencies where they meet. Often it is good practice to add in a Heater block with a temperature and pressure specification between the two sections with the different physical property methods. The Heater should use the temperature and pressure of the inlet stream and the physical property method of the new section or block to which the outlet from the Heater is connected. A Transfer block can be used to transfer the temperature and pressure of the inlet stream to the Heater block.

In this flowsheet, only the temperature is transferred since the pressures are all ambient. A similar transfer block could be used to transfer the pressure from the LIQUID2 stream to the TRANSFER Heater block.



Flowsheet variables from which information is copied

○ Entire stream

Stream name:

○ Stream flow

Stream name:

○ Substream

Stream name:

Substream:

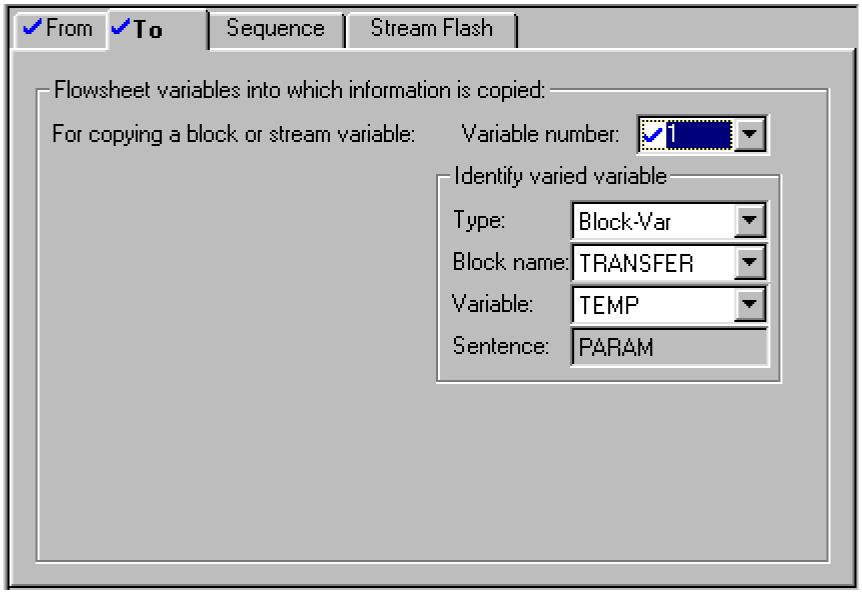
● Block or stream variable

Type: Stream-Var

Stream name: LIQUID2

Substream: MIXED

Variable: TEMP



Flowsheet variables into which information is copied:

For copying a block or stream variable: Variable number: ✓1

Identify varied variable

Type: Block-Var

Block name: TRANSFER

Variable: TEMP

Sentence: PARAM

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25 Balance Blocks

You can use a Balance block to calculate heat and material balances around an envelope of one or more unit operation blocks. The Balance block updates stream variables entering or leaving the envelope with the calculated results. For example, the Balance block can calculate:

- Flow rate of make-up streams in recycle calculations. (This eliminates Fortran blocks.)
- Feed stream flow rate and conditions, based on other stream and block information. (This eliminates design specifications and convergence loops.)

This chapter includes the following topics about Balance blocks:

- Defining a Balance block
- Specifying blocks and streams for balance calculations
- Specifying and updating stream variables
- Sequencing Balance blocks
- Flash specifications
- Material and energy balance equations

Defining a Balance Block

Define a Balance block by:

1. Creating the Balance block.
2. Specifying blocks and streams for balance calculations.
3. Specifying and updating stream variables.
4. Sequencing balance blocks.
5. Optionally, specifying flash conditions.

Creating a Balance Block

To create a Balance block:

1. From the Data menu, select Flowsheeting Options, then Balance.
2. On the Balance Object Manager, click the New button.
3. In the Create New ID dialog box, enter an ID or accept the Default ID and click OK.
4. Select the Balance form you want to enter data on from left pane of the Data Browser. See subsequent sections of this chapter for more information.

Form	Sheet	What is Specified
Setup	Mass Balance	Blocks or streams to include in each material balance envelope
	Energy Balance	Blocks or streams to include in each energy balance envelope
	Equations	Material and energy balance relationships in addition to what is specified on the Mass Balance and Energy Balance sheets
	Calculate	Stream variables to calculate and update after the mass and energy balance calculations
	Scale	Stream scale factors
Advanced	Parameters	Optional convergence parameters, including relative tolerance of balance equation residuals
	Sequence	Optional execution sequence for the balance block
	Stream Flash	Optional flash specifications for specified streams. This sheet can also be used to suppress automatic flash calculations for streams updated by the Balance block.
	Diagnostics	Levels of diagnostic output from the balance block

Specifying Blocks and Streams for Balance Calculations

Use the Mass Balance and Energy Balance sheets to specify blocks or streams for a mass and energy balance envelope. The energy balance equations are overall energy balances.

The mass balance equations can be any one of these:

- Overall. Do not specify Components, Component Groups, or Substreams.
- Substream. Do not specify Components or Component Groups.
- Component balances

To specify blocks or streams for mass balance calculations:

1. Select the Mass Balance sheet.
2. On the Mass Balance Number field, click the down arrow and select <new>.
3. In the New Item dialog box, specify an ID or accept the default ID. The ID must be an integer.
4. Specify blocks or streams (inlets and outlets) to include in the material balance envelope.
5. Specify components, component groups, or substreams, depending on the material balance type.
6. If you want to enter more than one material balance, repeat steps 2 through 5.

To specify blocks or streams for energy balance calculations:

1. Select the Energy Balance sheet.
2. On the Energy Balance Number field, click the down arrow and select <new>.
3. In the New Item dialog box, specify an ID or accept the default ID. The ID must be an integer.
4. Specify the blocks or streams (inlets and outlets) for the energy balance envelope.
5. If you want to enter more than one energy balance, repeat steps 2 through 4.

Tip If you want to delete an mass balance or energy balance, click the right mouse button on the Mass Balance Number or the Energy Balance Number field. From the popup menu, select Delete.

Use the Equations sheet to set up general molar/mass relationships among the total or component flows of one or more streams. You can also specify the mole and mass right hand side of a relation. See Material and Energy Balance Equations, this chapter, for more information about the form of the equations.

Specifying and Updating Stream Variables

Use the Calculate sheet to specify which stream variables to calculate by solving the mass and energy balance relationships. You can specify to update these variables after they are calculated. To solve the balance equations, the total number of variables specified on this form must equal the total number of equations specified on the Mass Balance and Energy Balance sheets.

Aspen Plus can calculate these types of flow variables:

- Total flow rate. The stream composition remains the same.
- Substream flow rates. The stream composition remains the same.
- Component flow rates of all applicable substream/component combinations

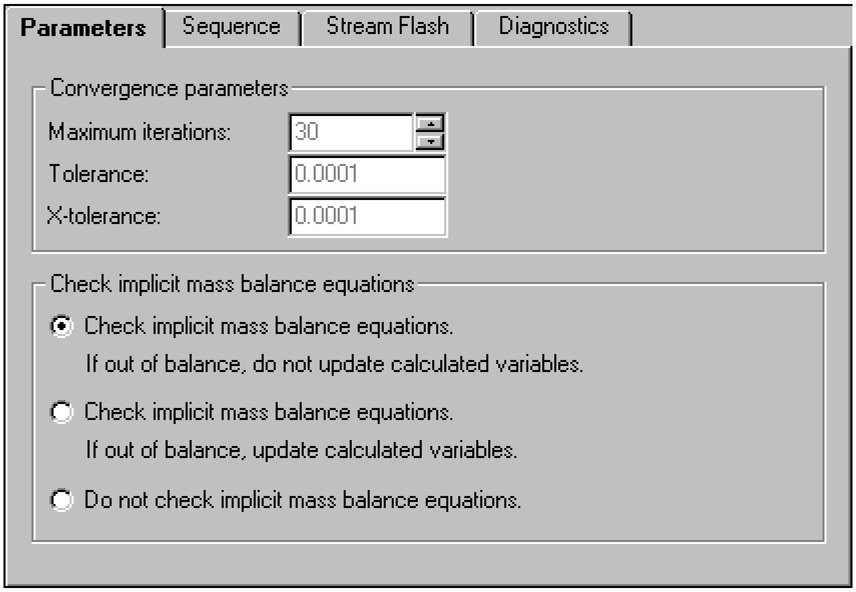
If you do not specify substreams when you specify component flows, Aspen Plus calculates the component flow rate of the default substream. The default substream for a specified component is the first substream containing that component.

Convergence Parameters

Use the Advanced Parameters sheet to:

- Specify Balance block convergence parameters
- Check additional implicit mass balance equations
- Adjust the maximum number of iterations, the relative tolerance of the balance equation residuals, and the relative tolerance of calculated variables

The implicit mass balance equations are any mass balance or mass/mole relationships which do not involve any variables to be calculated or material balance equations for the energy balance. The additional mass balance equations are checked by default, and if they are out of balance, the calculated variables are not updated. It is possible to update calculated variables even if the equations are out of balance. You can choose not to check the additional mass balance equations.



Convergence parameters

Maximum iterations: 30

Tolerance: 0.0001

X-tolerance: 0.0001

Check implicit mass balance equations

● Check implicit mass balance equations.
If out of balance, do not update calculated variables.

○ Check implicit mass balance equations.
If out of balance, update calculated variables.

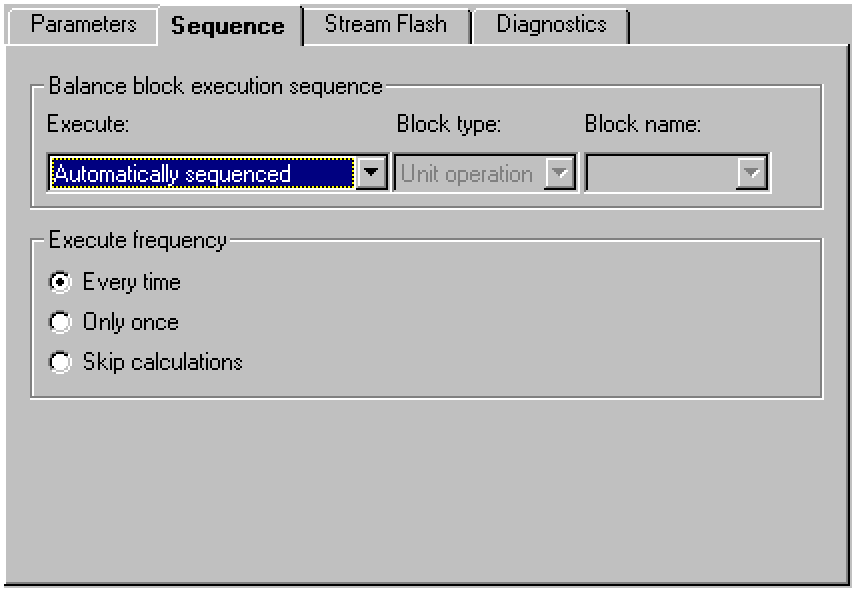
○ Do not check implicit mass balance equations.

Sequencing Balance Blocks

Use the Advanced Sequence sheet to specify when to execute a Balance block:

A Balance block can be sequenced automatically or manually. In automatic sequencing the Balance block executes before any unit operation block with a feed stream updated by this Balance block.

In some cases, Aspen Plus places the Balance block within a convergence loop. You can control whether the block executes only once (for example, for initializing a tear stream) or always (for example, for makeup calculations).



Balance block execution sequence

Execute: Automatically sequenced

Block type: Unit operation

Block name:

Execute frequency

● Every time

○ Only once

○ Skip calculations

Flash Specifications

Use the Stream Flash sheet to specify thermodynamic conditions or suppress automatic flash calculations for streams updated by a balance block. Aspen Plus automatically flashes an updated stream unless the only updated variable is the total flow.

Material and Energy Balance Equations

When the number of variables exceeds the number of equations, you must enter the unknown variables to be calculated on the Calculate form. Since the system of equations is linear, Aspen Plus solves the unknown variables directly. You can specify that the corresponding stream variables are updated.

Aspen Plus uses the following material and energy balance equations:

Overall mass balance:

$$\sum_{i=1}^{NM} S_i \sigma_i F_i = 0$$

Substream mass balance for j=1 to NSS:

$$\sum_{i=1}^{NM} S_i F_i f_{ij} = 0$$

Component mass balance for k=1 to NC, j=1 to NSS:

$$\sum_{i=1}^{NM} S_i F_i f_{ij} Z_{ijk} = 0$$

Overall energy balance:

$$\sum_{i=1}^{NM} S_i \sigma_i F_i h_i + \sum_{j=1}^{NH} S_j \sigma_j H_j + \sum_{k=1}^{NW} S_k \sigma_k W_k = RHS$$

Where:

S_i = +1 for inlet streams, -1 for outlet streams

σ_i = Stream scale factor

F_i = Mass flow of stream i

f_{ij} = Mass fraction of substream j in stream i

Z_{ijk} = Mass fraction of component k in substream j of stream i

NM = Number of combined inlet and outlet material streams

NH = Number of combined inlet and outlet heat streams

NW = Number of combined inlet and outlet work streams

NSS = Number of substreams within material streams

NC = Number of components specified on the Components Specifications or Components Comp-Group forms

h_i = Mass enthalpy of stream i

H_j = Heat flow of heat stream j

W_k = Work of work stream k

RHS = Right-hand side of the energy balance equation

On the Equations sheet, you can specify additional material relationships, which span components in various streams. This is useful for reactive systems. When you specify additional relationships, Aspen Plus uses the following mole/mass balance equations for the component mole/mass balance equation:

$$\sum_{j=1}^{NT_i} C_{ij} F_{ij} = RHS_i$$

Where:

C_{ij} = Coefficient of Term j in equation i

F_{ij} = Mole/mass flow Term j in equation i as determined by Stream, Substream, and Component of the term

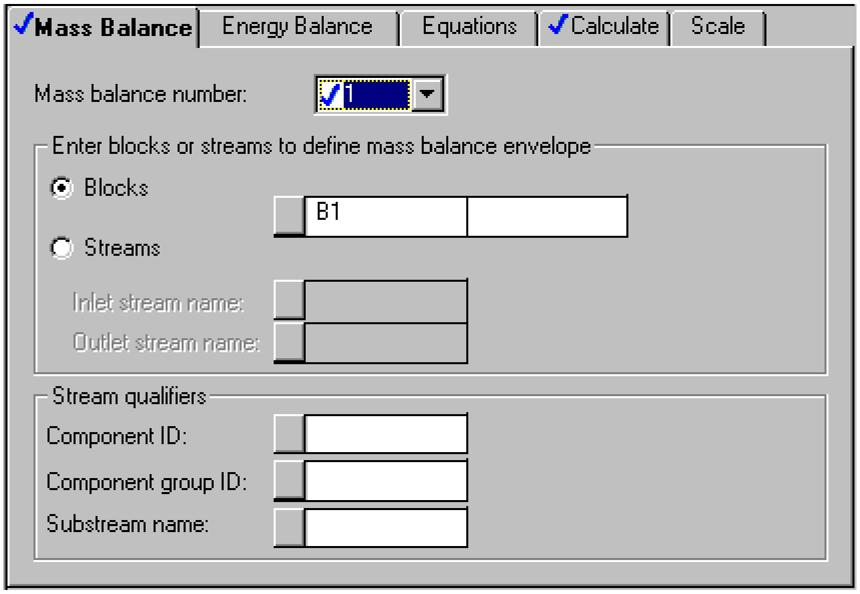
RHS_i = Right-hand side of mole/mass equation i

NT_i = Number of terms in mole/mass equation i

Example of Backward Calculations Using a Balance Block

This example shows how to do a mass-only calculation around a HeatX block. The objective is to demonstrate the capability of a balance block to do backward calculations.

Flow rates of the two outlet streams from HeatX are given. Flow rates of the two inlet streams into HeatX need to be calculated. Both the inlet and the outlet streams are specified, but the flow rates specified for the two inlets are just dummy numbers.



Mass balance number: ✓1

Enter blocks or streams to define mass balance envelope

● Blocks: B1

○ Streams

Inlet stream name:

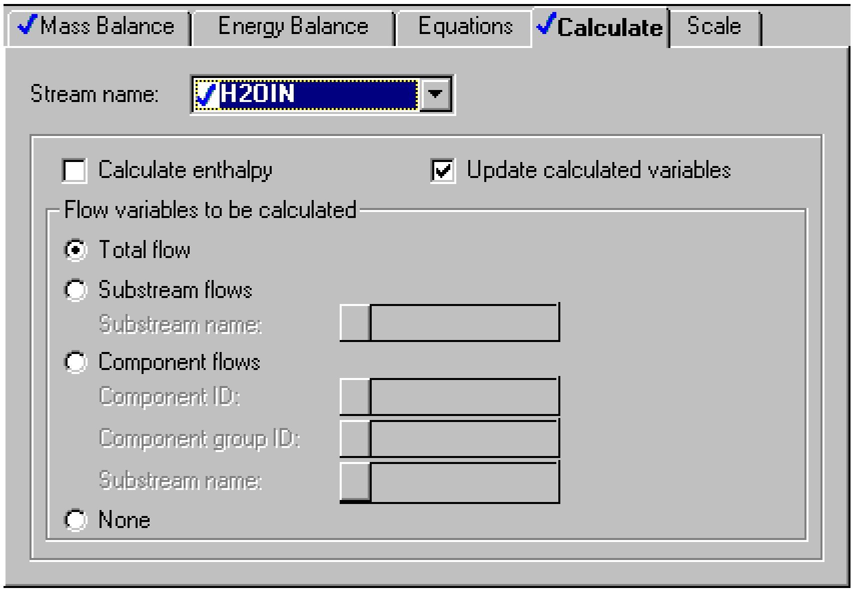
Outlet stream name:

Stream qualifiers

Component ID:

Component group ID:

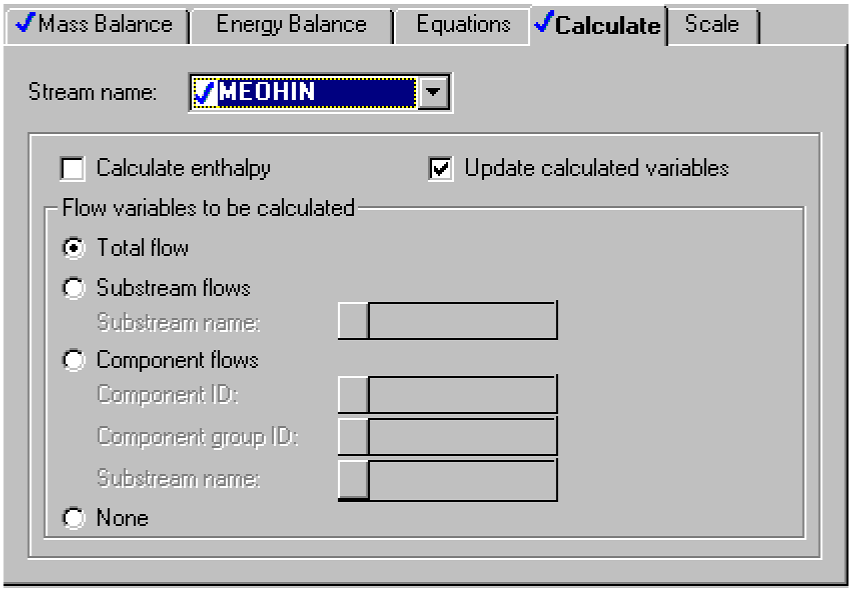
Substream name:



Stream name: ✓H2OIN

☐ Calculate enthalpy
☑ Update calculated variables

Flow variables to be calculated
- ● Total flow
- ○ Substream flows
  - Substream name:
- ○ Component flows
  - Component ID:
  - Component group ID:
  - Substream name:
- ○ None



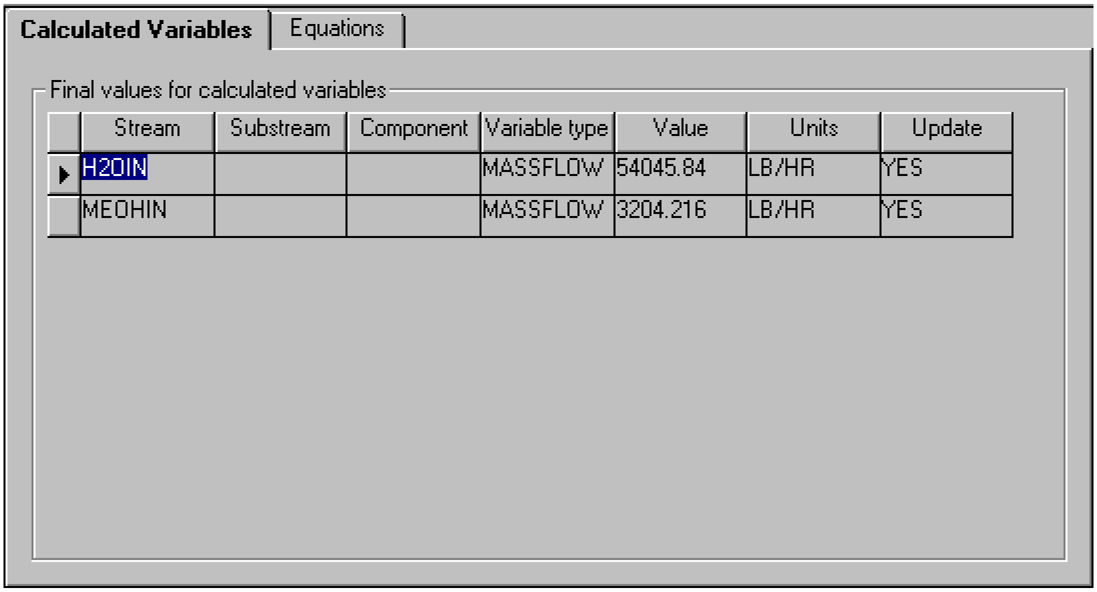
Stream name: ✓MEOHIN

☐ Calculate enthalpy
☑ Update calculated variables

Flow variables to be calculated
- ● Total flow
- ○ Substream flows
  - Substream name:
- ○ Component flows
  - Component ID:
  - Component group ID:
  - Substream name:
- ○ None

On the results form, the final values for the calculated variables and for the balance equations are tabulated.

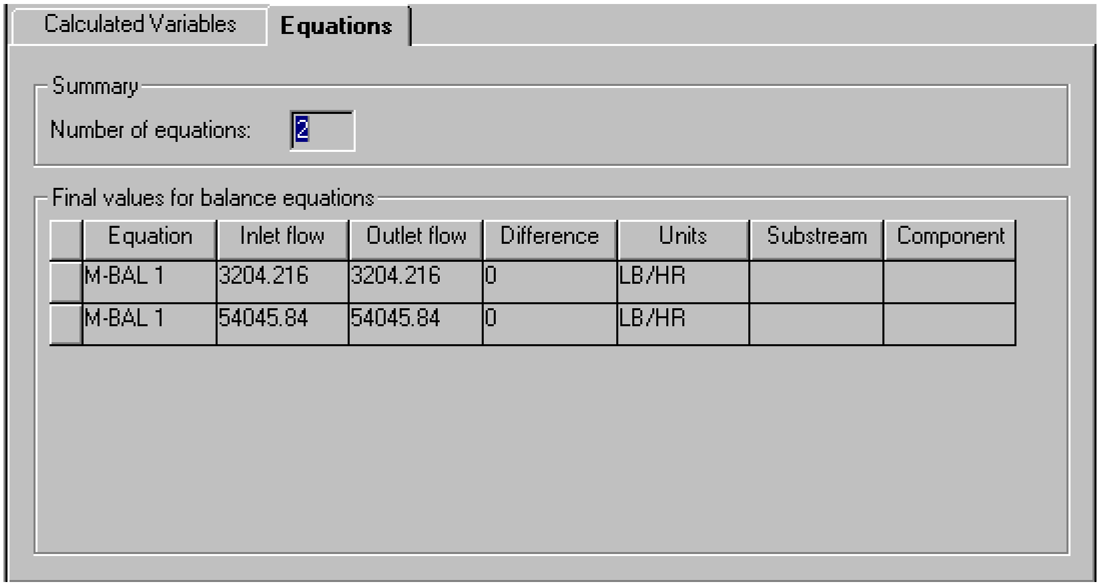
The final values for the calculated variables are found on the Calculated Variables sheet. In this example, the mass flow of the two inlet streams, H2OIN and MECHIN are calculated.



Final values for calculated variables

Stream	Substream	Component	Variable type	Value	Units	Update
H2OIN			MASSFLOW	54045.84	LB/HR	YES
MEOHIN			MASSFLOW	3204.216	LB/HR	YES

The final values for the balance equations are found on the Equations sheet. The number of equation in the problems is shown; here there are two mass balance equations.



Summary

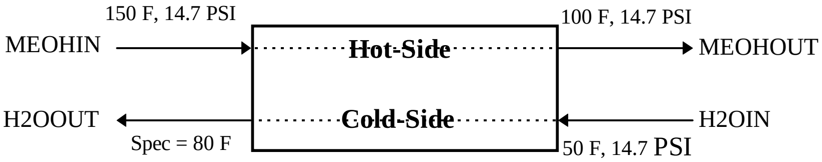
Number of equations: 2

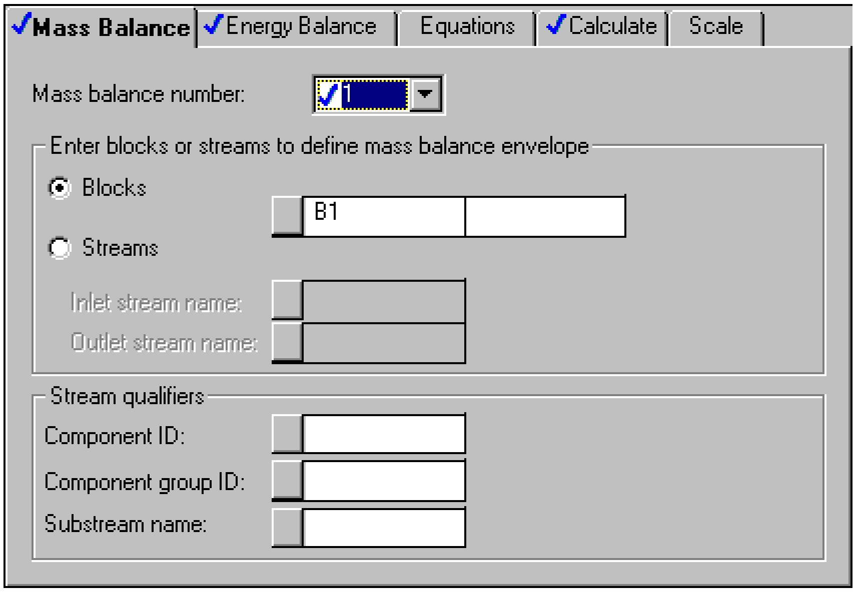
Final values for balance equations

Equation	Inlet flow	Outlet flow	Difference	Units	Substream	Component
M-BAL 1	3204.216	3204.216	0	LB/HR		
M-BAL 1	54045.84	54045.84	0	LB/HR		

Example of Calculating a Coolant Flow Rate

Use a balance block to calculate the required flow rate of cooling water in order to cool a stream of methanol from 150 F to 100 F. A Balance block will eliminate the need for a Design specification and a convergence loop.





Mass balance number: ✓1

Enter blocks or streams to define mass balance envelope

● Blocks B1

○ Streams

Inlet stream name:

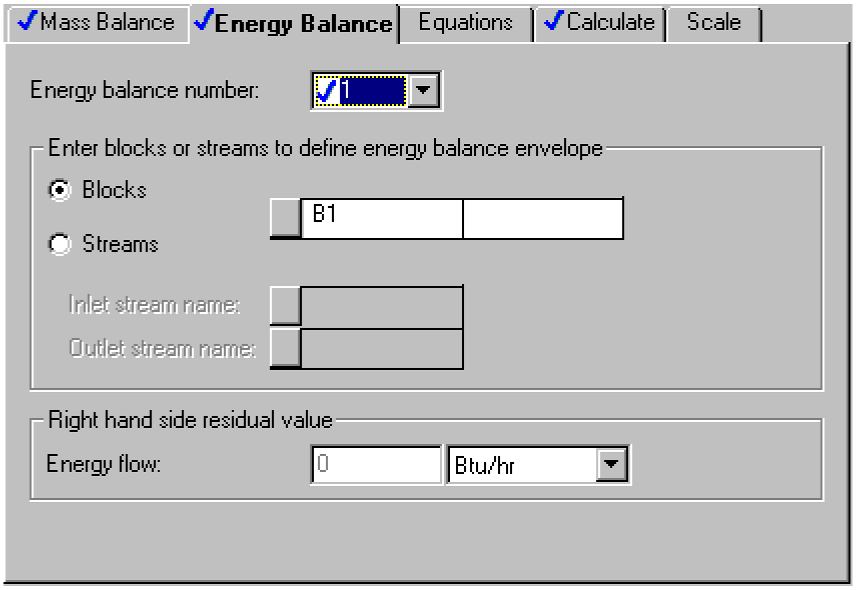
Outlet stream name:

Stream qualifiers

Component ID:

Component group ID:

Substream name:



Energy balance number: ✓1

Enter blocks or streams to define energy balance envelope

● Blocks B1

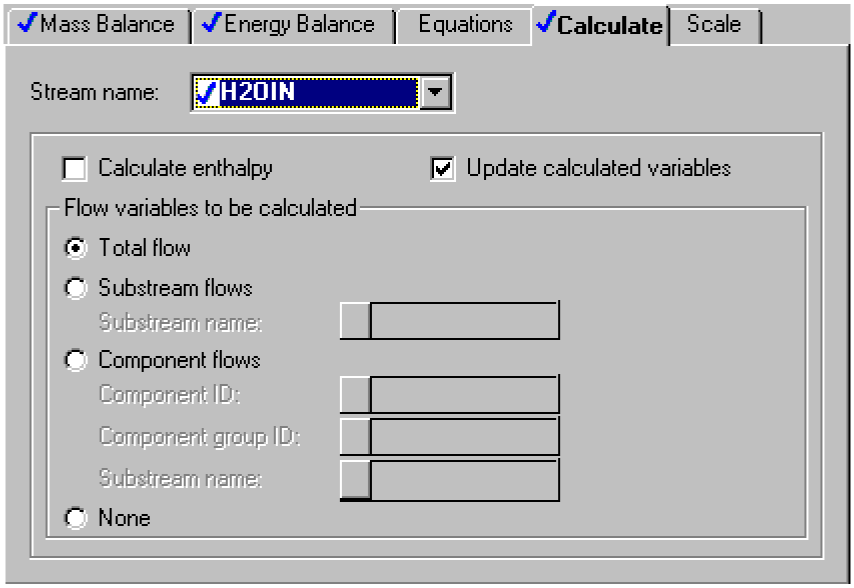
○ Streams

Inlet stream name:

Outlet stream name:

Right hand side residual value

Energy flow: 0 Btu/hr



Stream name: ✓H2OIN

☐ Calculate enthalpy ☑ Update calculated variables

Flow variables to be calculated

● Total flow

○ Substream flows

Substream name:

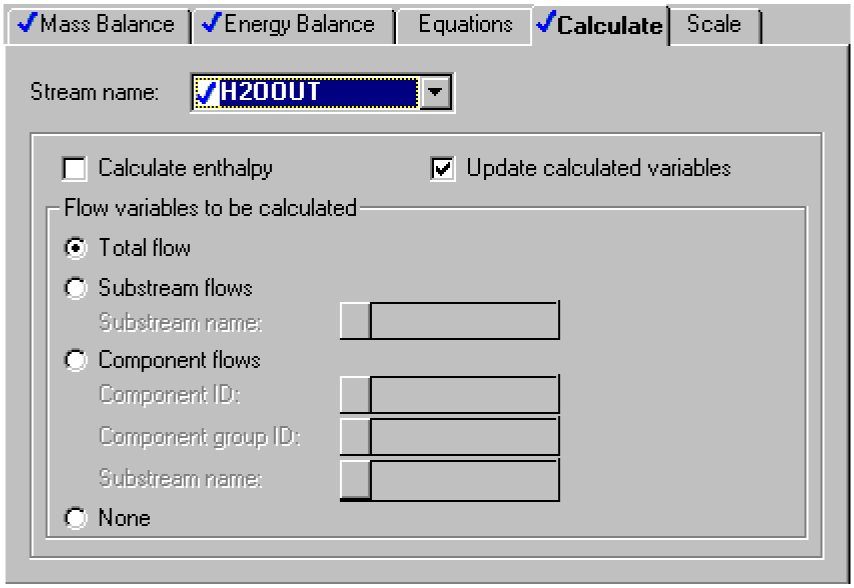
○ Component flows

Component ID:

Component group ID:

Substream name:

○ None



Stream name: ✓H2OOUT

☐ Calculate enthalpy ☑ Update calculated variables

Flow variables to be calculated

● Total flow

○ Substream flows

Substream name:

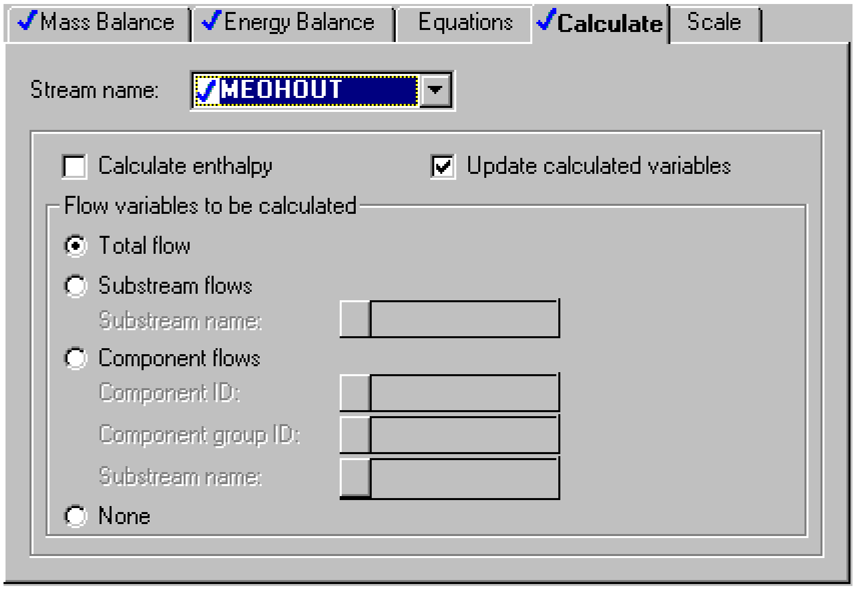
○ Component flows

Component ID:

Component group ID:

Substream name:

○ None



Stream name: ✓MEOHOUT

☐ Calculate enthalpy ☑ Update calculated variables

Flow variables to be calculated

● Total flow

○ Substream flows

Substream name:

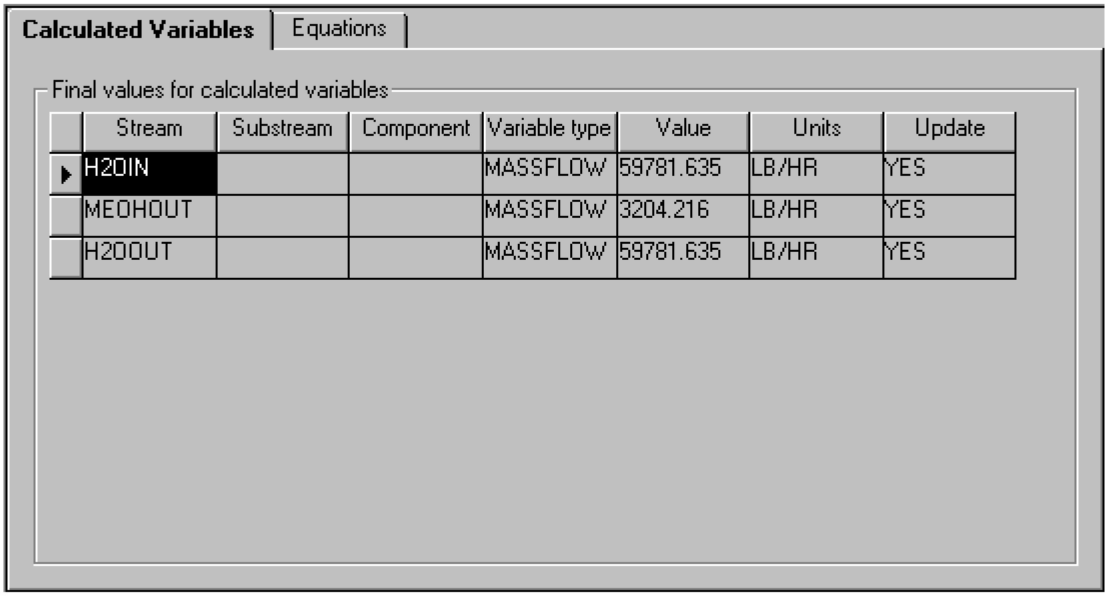
○ Component flows

Component ID:

Component group ID:

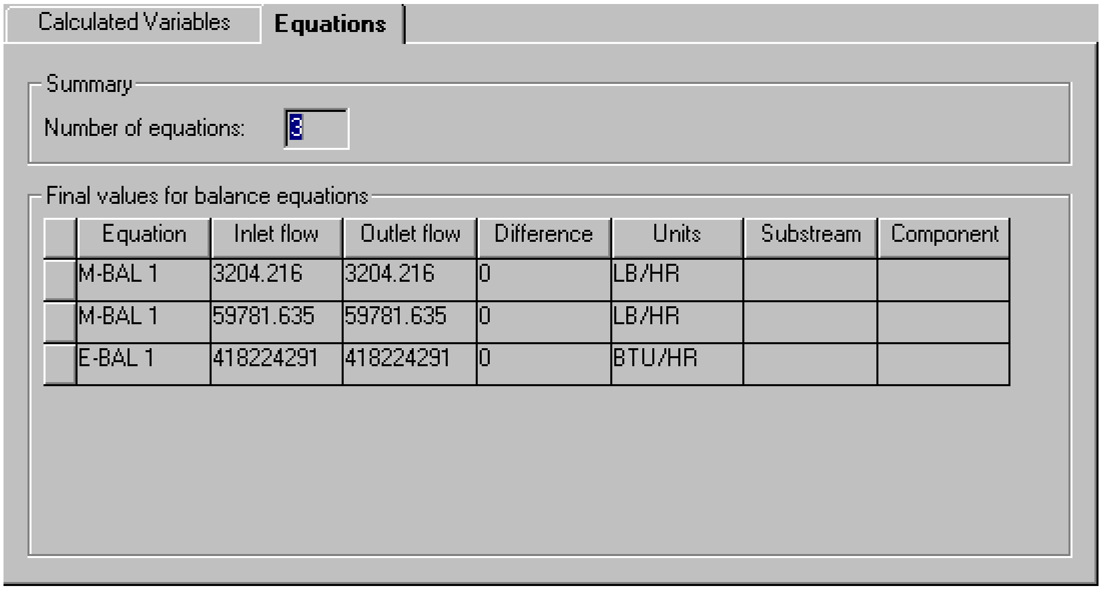
Substream name:

○ None



Final values for calculated variables

Stream	Substream	Component	Variable type	Value	Units	Update
H2OIN			MASSFLOW	59781.635	LB/HR	YES
MEOHOUT			MASSFLOW	3204.216	LB/HR	YES
H2OOUT			MASSFLOW	59781.635	LB/HR	YES



Summary

Number of equations: 3

Final values for balance equations

Equation	Inlet flow	Outlet flow	Difference	Units	Substream	Component
M-BAL 1	3204.216	3204.216	0	LB/HR		
M-BAL 1	59781.635	59781.635	0	LB/HR		
E-BAL 1	418224291	418224291	0	BTU/HR		

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26 Case Study

This chapter includes information about:

- Using Case Study
- Creating a Case Study
- Identifying Case Study variables
- Specifying values for Case Study variables
- Specifying report options for Case Study

Using Case Study

After you run a base-case simulation, you may want to run several parametric cases for the same flowsheet. You can use the Case Study tool to run multiple simulation cases for the same flowsheet when you make batch runs. Case Study will perform a flowsheet simulation for each case in a series. The Case Study block does not affect the base-case simulation or the base-case report.

Aspen Plus generates a report for each case. You can tailor the case reports to contain only those report sections of interest.

Aspen Plus ignores a Case Study block when you make interactive runs from the user interface. See Chapter 11, Running Your Simulation for more information on batch runs.

Creating a Case Study

To create a Case Study:

1. From the Data menu, point to Model Analysis Tools, then Case Study.

2. On the Case Study Setup Vary sheet, identify the variables you want to change from case to case. See Identifying Case Study Variables, this chapter.
3. On the Case Study Setup Specifications sheet, specify values for the case study variables for each case. See Specifying Values for Case Study Variables, this chapter.
4. If you want to specify report options, use the Case Study ReportOptions form. See Specifying Report Options for Case Studies, this chapter.

Identifying Case Study Variables

Use the Case Study Setup Vary sheet to identify flowsheet variables you want to change from case to case. You can only change block input, process feed stream, and other input variables. Result variables cannot be modified directly.

To identify the variables you want to change from case to case:

1. On the Case Study Setup form, select the Vary tab.
2. On the Variable Number field, click the down arrow and select <new> from the list.
3. In the Manipulated Variable Type field, select a variable type.
4. Aspen Plus automatically shows the fields necessary to uniquely identify the flowsheet variables. Complete the fields to define the variable. See Chapter 18, Accessing Flowsheet Variables, for more information on accessing variables.
5. You have the option of labeling the variables for the report. Use the Report Labels Line 1 to Line 4 fields to define these labels.
6. Repeat steps 2-5 until you have identified all case study variables.

Specifying Values for Case Study Variables

Use the Case Study Setup Specifications sheet to specify values for the case study variables.

To specify values for case study variables:

1. On the Case Study Setup form, select the Specifications tab.

2. On the Case Number field, click the down arrow and select <new> from the list.
3. In the New Item dialog box, enter an ID or accept the default ID. The ID must be an integer.
4. In the Values for Manipulated Variable field, enter a value for each variable. Enter multiple variable values in the same order as you identified them on the Vary sheet.
5. To enter another case, repeat steps 2 and 3 until you have defined all the cases you want to run.

On the Case Study Setup Specifications sheet, you can also:

- Reset convergence and unit operation restart flags for blocks
- Restore initial values for tear streams and feed streams
- Enter the case report description

Resetting Initial Values

Use the Case Study Setup Specifications sheet to reset convergence and unit operation reinitialization options for blocks. You can also restore initial values for tear streams, feed streams manipulated by design specifications, optimization blocks, and Fortran blocks. By default, blocks or streams are not reinitialized. It is usually most efficient to begin the calculation for a new case with the results of the previous case.

To reinitialize blocks:

1. On the Case Study Setup form, select the Specifications tab.
2. In the Blocks to be Reinitialized field, select either Include Specified Blocks or Reinitialize All Blocks.
3. If you choose Include Specified Blocks, select the unit operation blocks and/or the convergence blocks to be reinitialized.

To reinitialize streams:

1. On the Case Study Setup form, select the Specifications tab.
2. In the Streams to be Reinitialized field, select either Include Specified Streams or Reinitialize All Streams.
3. If you choose Include Specified Streams, select the streams to be reinitialized.

Entering a Description

Use the Case Study Setup Specifications sheet to enter the case report description, which will appear as a title in the case report.

To enter a case report description:

1. On the Case Study Setup form, select the Specifications tab.
2. Click the Description button.
3. Enter the description.
4. Click Close.

Specifying Report Options for Case Studies

Use the Case Study ReportOptions form to specify which sections of the report to include or suppress in the case reports. A separate report is generated for each case and appended to the report file. If you specified report options for the base case on the Setup ReportOptions form, and would like the same options for the case reports, you must re-specify the report options on the Case Study ReportOptions sheet.

Any options for Block reports which you specified for the base case on the Setup ReportOptions Block sheet or on the BlockOptions ReportOptions sheet for the block also applies to the case reports.

The following table shows what you can specify and where:

To specify	ReportOptions Sheet
Whether to generate a report file and which sections of the report to include	General
Which flowsheet option reports to include in the report file	Flowsheet
Which block reports to include in the report file	Block
Which streams to include in the report file and the format for the streams	Stream
Whether to generate additional stream reports, and if so the streams to include in the report file and the format for the streams	Supplementary Stream

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27 Specifying Reactions and Chemistry

This chapter describes how to define reaction systems in Aspen Plus including:

- About Reactions and Chemistry
- About Electrolytes Chemistry
- Specifying Electrolytes Chemistry
- Specifying Power Law Reactions for Reactors and Pressure Relief Systems
- Reactions With Solids
- Specifying LHHW Reactions for Reactors and Pressure Relief Systems
- Specifying Reactions for Reactive Distillation
- Using a User Kinetic Subroutine

About Reactions and Chemistry

There are two types of reaction systems and Aspen Plus uses different methods for simulating them:

Type of reaction system	Description	Use this Data Browser Form
Electrolytes solution chemistry	Reactions involving the formation of ionic species	Chemistry
Non-electrolyte reactions	Rate-controlled or equilibrium limited. For reactors and reactive distillation modeling.	Reactions

Reactions

Rate-controlled and non-electrolyte equilibrium reactions are specified as Reaction IDs that can be referenced in kinetic reactors, columns, and pressure relief calculations. These reactions can be used by:

- RadFrac, RateFrac, and BatchFrac for reactive distillation
- RBatch, RCSTR, and RPlug, the kinetics-based reactor models
- Pressure Relief model for pressure relief calculations in reactive systems

The reaction kinetics of rate-based reactions can be represented using any of the following expressions:

- Power Law kinetic model
- Langmuir-Hinshelwood-Hougen-Watson (LHHW) kinetic model (not applicable to reactive distillation systems)
- User-defined kinetic model

Chemistry

Electrolyte solution chemistry is specified as a Chemistry ID that can be referenced on the Properties Specification Global sheet and on the BlockOptions Properties sheets for individual unit operation blocks. Unlike non-electrolyte reactions which are specified and executed only within certain unit operation blocks and pressure relief calculations, electrolyte chemistry definitions become part of the physical property specifications for a simulation or flowsheet section. They are used for all calculations (in any stream or unit operation block) which use that property specification.

About Electrolytes Chemistry

In electrolyte systems, molecular species dissociate partially or completely in solution and/or precipitate as salts. Examples include the following systems:

- Sour water (H_2S-NH_3-CO_2-Water)
- Amines
- Acids (HCl-Water)
- Brine (NaCl-Water)

Electrolyte systems are characterized by their base molecular components (the apparent components), and by:

- Species resulting from dissociation and/or precipitation, such as ions and salts
- Compounds formed through chemical reactions among the species

There are three types of electrolyte reactions:

Type	Example
Partial dissociation equilibria [†]	$HCl + H_2O \leftrightarrow H_3O^+ + Cl^-$
Salt precipitation equilibria [†]	$NaCl$ (Salt) $\leftrightarrow Na^+ + Cl^-$
Complete dissociation	$NaCl$ (liquid phase) $\rightarrow Na^+ + Cl^-$

[†] *Equilibrium constants are required to model these reactions. They can be calculated from correlations (as a function of temperature) or from Gibbs free energy.*

Collectively the species and reactions are referred to as the electrolytes chemistry. Electrolytes chemistry must be modeled correctly for accurate simulation results. Normally this requires expert knowledge of the solution chemistry. In most cases, however, the Aspen Plus Electrolytes Wizard can generate the species and reactions for you, using a built-in knowledge base of reactions, equilibrium constant data, and possible ionic species. For more information on the Electrolytes Wizard, see Chapter 6.

Specifying Electrolytes Chemistry

To specify the electrolytes chemistry for a simulation, you must:

1. Define the complete set of components present (including ions, salts, and other species generated by reaction) on the Components Specification Selection sheet.

2. Define the stoichiometry and reaction type, using the Reactions Chemistry Stoichiometry sheet.

3. Specify the concentration basis, the temperature approach to equilibrium, and coefficients for the equilibrium constant expression, using the Reactions Chemistry EquilibriumConstants sheet.

It is recommended that you use the Electrolytes Wizard to define both the components and reactions. The Electrolytes Wizard:

- Uses a built-in knowledge base to generate the electrolyte components and reactions
- Accesses the Aspen Plus electrolytes reaction database for equilibrium constant data

For information on the Electrolytes Wizard, see Chapter 6.

You can define your own electrolyte chemistry, or you can view or modify the chemistry generated by the Electrolytes Wizard.

To define, view, or modify electrolyte chemistry:

1. From the Data menu, point to Reactions then Chemistry.
2. To create a new Chemistry ID, click New on the Reactions Chemistry Object Manager. Enter an ID in the Create new ID dialog box or accept the default ID, and click OK.
3. To modify an existing Chemistry ID, select its name in the Object Manager and choose Edit.
4. Follow the instructions in subsequent sections of this chapter for details on defining each type of reaction within a Chemistry ID.

The following sections explain how to create new reactions within an existing Chemistry ID, by specifying stoichiometry and calculations options for the equilibrium constant. You can specify any number of reactions within a Chemistry ID.

You also can have any number of Chemistry IDs in your simulation. Because the Chemistry ID becomes part of the total Property Method definition, you can specify different Chemistry IDs anywhere you use different Property Methods, such as flowsheet sections or individual unit operation blocks. For more information on specifying multiple Property Methods within a flowsheet, see Chapter 7.

Defining Stoichiometry for Electrolytes Chemistry

Equilibrium Ionic Reactions

Equilibrium ionic reactions describe the partial dissociation of weak electrolytes and other liquid phase equilibria. Each equilibrium ionic reaction within a Chemistry ID is referenced with a reaction number (for example, 1, 2, 3, etc.)

To define a new reaction number and specify the stoichiometry for an ionic equilibrium reaction:

1. On the Reactions Chemistry Stoichiometry sheet for your Chemistry ID, click New.
2. On the Select Reaction Type dialog box, Equilibrium is the default reaction type. Enter an ID or accept the default ID and click OK. The ID must be an integer.
3. On the Equilibrium Reaction Stoichiometry dialog box, enter the components and stoichiometric coefficients that make up your reaction. Coefficients should be negative for reactants and positive for products.
4. Click Close when finished. You should see your new reaction listed on the Stoichiometry sheet with the information displayed in equation form.
5. Repeat steps 1-4 for each additional ionic equilibrium reaction.

Salt Precipitation Reactions

Salt precipitation reactions describe the formation or dissolution of salts in equilibrium with the liquid phase. Each salt precipitation reaction within a Chemistry ID is referenced by the component name of the salt.

To define the stoichiometry for a new salt precipitation reaction:

1. On the Reactions Chemistry Stoichiometry sheet for your Chemistry ID, click New.
2. On the Select Reaction Type dialog box, select Salt in the Choose Reaction Type frame.
3. In the Enter Salt Component ID field, select the name of the salt for which you are defining the reaction, and click OK.
4. On the Salt Dissolution Stoichiometry dialog box, enter the components and stoichiometric coefficients for the products (ions) formed by the dissolution of the salt.
5. Click Close when finished. You should see your new reaction listed on the Stoichiometry sheet with the information displayed in equation form.
6. Repeat steps 1-5 for each additional salt precipitation reaction.

Complete Dissociation Reactions

Complete dissociation reactions describe the complete dissociation of strong electrolytes in the liquid phase. These reactions do not have equilibrium constants. Each complete dissociation reaction within a Chemistry ID is referenced by the name of the dissociating component.

To define the stoichiometry for a new complete dissociation reaction:

1. On the Reactions Chemistry Stoichiometry sheet for your Chemistry ID, click New.
2. On the Select Reaction Type dialog box, select Dissociation in the Choose Reaction Type frame.
3. In the Enter Dissociating Electrolyte field, select the name of the component for which you are defining the reaction, and click OK.
4. On the Electrolyte Dissociation Stoichiometry dialog box, enter the components and stoichiometric coefficients for the dissociation products.
5. Click Close when finished. You should see your new reaction listed on the Stoichiometry sheet with the information displayed in equation form.
6. Repeat steps 1-5 for each additional complete dissociation reaction.

Defining Equilibrium Constants for Electrolytes Chemistry

Equilibrium constants are required to model equilibrium ionic reactions and salt precipitation reactions. Aspen Plus can calculate these equilibrium constants from correlations (as a function of temperature) or from reference state Gibbs free energy (available in the Aspen Plus databanks).

To define how the equilibrium constants will be calculated for the equilibrium ionic reactions and salt precipitation reactions within your Chemistry ID:

1. On the Reactions Chemistry form for your Chemistry ID, select the Equilibrium Constants sheet.
2. Choose the concentration basis for equilibrium constants in the Concentration Basis For Keq list. The concentration basis determines how the equilibrium constant is calculated:

Concentration Basis	**Equilibrium Constant Definition** [†]
Mole-Frac (default)	$K = \Pi(x_i \gamma_i)^{\nu_i}$
Molal	$K = \Pi(m_i \gamma_i)^{\nu_i}$

[†] Where:

K = Equilibrium constant
x = Component mole fraction
m = Molality (gmole/kg-H_2O)
γ = Activity coefficient
ν = Stoichiometric coefficient
i = Component index
Π is the product operator.

All properties refer to the liquid phase.

3. You can specify a Temperature Approach to Equilibrium that applies to all ionic equilibrium and salt precipitation reactions defined in the Chemistry ID. The temperature approach you specify is added to the stream or block temperature to compute the equilibrium constants. If you do not specify a temperature approach, Aspen Plus uses a default value of 0.
4. Use the Hydrate-Check field to select the method that Aspen Plus uses to determine which hydrate to precipitate when you have specified multiple hydrates as precipitation reactions for a salt.

Hydrate-check Method	Information
Rigorous (default)	Uses Gibbs free energy minimization to select the hydrate. Allows Aspen Plus to predict the formation of the correct hydrate for salts with multiple hydrates.
Approximate	Uses the lowest solubility product value at the system temperature to select the hydrate. Requires less computation time than the rigorous method.

5. Select the appropriate reaction type (Equilibrium Reaction or Salt), and choose the appropriate reaction from the list.
6. Leave the equilibrium coefficients blank.

   – or –

   Enter coefficients for the built-in equilibrium constant expression:
   $\ln (Keq) = A + B / T + C*ln (T) + D*T$

   Where:

   Keq = Equilibrium constant
   T = Temperature in Kelvin
   A, B, C, D = User supplied coefficients

   The definition of K depends on the concentration basis selected.

   If coefficients are not entered, Aspen Plus computes the equilibrium constant from the reference state Gibbs free energies of formation.

Repeat steps 5 and 6 for all ionic equilibrium reactions and salt precipitation reactions included in the Chemistry ID. Because complete dissociation reactions do not have equilibrium constants, nothing on the Equilibrium Constants sheet applies to reactions of this type.

Specifying Power Law Reactions for Reactors and Pressure Relief Systems

Powerlaw Reaction IDs can represent equilibrium reactions, or rate-controlled reactions represented by the power law. To use a Powerlaw Reaction ID in the Aspen Plus reactor models RCSTR, RPlug, and RBatch, or for the pressure relief calculations in Pres-Relief, you need to:

- Define the type and stoichiometry of the reactions
- Enter equilibrium or kinetic parameters

RPlug, RBatch, and Pres-Relief can handle rate-controlled reactions. RCSTR can handle both rate-controlled and equilibrium reactions.

To create a new Powerlaw Reaction ID:

1. From the Data menu, point to Reactions then Reactions.
2. To create a new Reaction ID, click New in the Reactions Object Manager.
3. In the Create New ID dialog box, enter a reaction ID in the Enter ID field, or accept the default ID.
4. Select Powerlaw in the Select Type list, and click OK.

   Once the Reaction ID is created, Aspen Plus brings you to the Stoichiometry sheet where you can begin defining reactions within the Reaction ID. There are two types of reactions allowed in a Powerlaw type Reaction ID.

Type	For
Equilibrium	Equilibrium reactions
Kinetic	Rate-controlled reactions

5. To specify the individual reactions within your reaction ID, follow the instructions in subsequent sections of this chapter for the type of reaction you want to create.

Equilibrium Reactions (for RCSTR only)

To add equilibrium type reactions to your Powerlaw Reaction ID:

1. Click New on the Reactions Stoichiometry sheet of your Powerlaw Reaction ID.

2. On the Edit Reaction dialog box, select Equilibrium from the Reaction Type list. The reaction number is entered automatically.
3. Enter components and stoichiometric coefficients to define the reaction. Coefficients should be negative for reactants and positive for products. You should not specify exponents for equilibrium reactions.
4. Click Close when finished. You should see your new reaction number, type, and equation displayed on the Stoichiometry sheet.
5. Repeat steps 1 through 4 for each additional equilibrium reaction.
6. Select the Equilibrium tab on the Reactions form to open that sheet.
7. On the Equilibrium sheet, select a reaction from the list at the top of the sheet.
8. Specify the phase in which the reaction will occur in the Reacting Phase list. The default is the liquid phase.
9. If the reaction does not actually reach equilibrium, you can enter a temperature approach to equilibrium in the Temperature Approach to Equilibrium field. The number of degrees you enter will be added to the reactor temperature to compute the equilibrium constant.
10. Choose whether you want to compute Keq from Gibbs energies or from a built in polynomial expression by selecting the appropriate option.

    If you choose Compute Keq From Gibbs Energies, you do not need to enter coefficients for the equilibrium constant. Aspen Plus will compute the Keq from the reference state Gibbs free energy of the components.
11. If you choose Compute Keq From Built-In Expression, enter coefficients for the built-in equilibrium constant expression, and choose a basis for the equilibrium constant:

    $\ln Keq = A + B/T + C*\ln(T) + D*T$

    Where:

    Keq = Equilibrium constant

    T = Temperature in Kelvin

    A, B, C, D = User-supplied coefficients

The definition of *Keq* depends on the basis you select in the Keq Basis list.

Keq Basis	**Equilibrium Constant Definition**[†]
Mole gamma (default)	$Keq = \Pi (x_i \gamma_i)^{\upsilon_i}$ (liquid only)
Molal gamma	$Keq = \Pi (m_i \gamma_i)^{\upsilon_i}$ (electrolytes, liquid only)
Mole fraction	$Keq = \Pi (x_i)^{\upsilon_i}$
Mass fraction	$Keq = \Pi (x_i^m)^{\upsilon_i}$
Molarity	$Keq = \Pi (C_i)^{\upsilon_i}$
Molality	$Keq = \Pi (m_i)^{\upsilon_i}$ (liquid only)
Fugacity	$Keq = \Pi (f_i)^{\upsilon_i}$
Partial pressure	$Keq = \Pi (p_i)^{\upsilon_i}$ (vapor only)
Mass concentration	$Keq = \Pi (C_i^m)^{\upsilon_i}$

[†] Where:

Keq = Equilibrium constant
x = Component mole fraction
x^m = Component mass fraction
C = Molarity (kgmole/m^3)
m = Molality (gmole/kg-H_2O)
γ = Activity coefficient
f = Component fugacity (N/m^2)
p = Partial pressure (N/m^2)
C^m = Mass concentration (kg/m^3)
υ = Stoichiometric coefficient (positive for products, negative for reactants)
i = Component index
Π is the product operator

12. If solids are present, click the Solids button and select the appropriate options for calculation of concentration. For more information, see Reactions With Solids, this chapter.
13. Repeat steps 7 through 12 for each equilibrium reaction.

Rate-Controlled Reactions

To add kinetic type reactions to your Powerlaw Reaction ID:

1. Click New on the Reactions Stoichiometry sheet of your Powerlaw Reaction ID.
2. On the Edit Reaction dialog box, Reaction Type defaults to Kinetic, and the reaction number is entered automatically. Enter components and stoichiometric coefficients to define the reaction. Coefficients should be negative for reactants and positive for products.

3. Specify power law exponents for the components. These exponents represent the *order* of the reaction with respect to each component. If you do not specify an exponent for a component, Aspen Plus uses a default value of 0.
4. Click Close when finished. You should see your new reaction number, type, and equation displayed on the Stoichiometry sheet.
5. Repeat steps 1 through 4 for each additional kinetic reaction.
6. Select the Kinetic sheet.
7. On the Kinetic sheet, select a reaction from the list at the top of the sheet.
8. Specify in which phase the reaction will take place in the Reacting Phase field. The default is the liquid phase.
9. Enter the pre-exponential factor (k), the temperature exponent (n), and the activation energy (E) in the appropriate fields. The pre-exponential factor must be in the SI units described later in this section. The temperature exponent refers to temperature in Kelvin.
10. In the [Ci] Basis list, select the concentration basis. The concentration basis determines which form of the power law expression will be used, as discussed later in this section.
11. If solids are present, click the Solids button and select the appropriate options for calculation of concentration. For more information, see Reactions With Solids, this chapter.
12. Repeat steps 7 through 11 for each kinetic reaction.

The power law expression depends on the concentration basis you select in the [Ci] Basis list:

[Ci] Basis	**Power Law Expression[†] (To is not specified)**	**Power Law Expression[†] (To is specified)**
Molarity (default)	$r = kT^n e^{-E/RT} \Pi (C_i)^{\alpha_i}$	$r = k (T/To)^n e^{(-E/R)[1/T-1/To]} \Pi (C_i)^{\alpha_i}$
Molality(electrolytes only)	$r = kT^n e^{-E/RT} \Pi (m_i)^{\alpha_i}$	$r = k (T/To)^n e^{(-E/R)[1/T-1/To]} \Pi (m_i)^{\alpha_i}$
Mole fraction	$r = kT^n e^{-E/RT} \Pi (x_i)^{\alpha_i}$	$r = k (T/To)^n e^{(-E/R)[1/T-1/To]} \Pi (x_i)^{\alpha_i}$
Mass fraction	$r = kT^n e^{-E/RT} \Pi (x_i^m)^{\alpha_i}$	$r = k (T/To)^n e^{(-E/R)[1/T-1/To]} \Pi (x_i^m)^{\alpha_i}$
Partial pressure(vapor only)	$r = kT^n e^{-E/RT} \Pi (p_i)^{\alpha_i}$	$r = k (T/To)^n e^{(-E/R)[1/T-1/To]} \Pi (p_i)^{\alpha_i}$
Mass concentration	$r = kT^n e^{-E/RT} \Pi (C_i^m)^{\alpha_i}$	$r = k (T/To)^n e^{(-E/R)[1/T-1/To]} \Pi (C_i^m)^{\alpha_i}$

[†] *Where:*
r = *Rate of reaction*
k = *Pre-exponential factor*
T = *Temperature in degrees Kelvin*
To = *Reference temperature in degrees Kelvin*
n = *Temperature exponent*
E = *Activation energy*
R = *Universal gas law constant*
x = *Mole fraction*
x^m = *Mass fraction*
C = *Molarity* $(kgmole/m^3)$
m = *Molality* $(gmole/kg\text{-}H_2O)$
C^m = *Mass concentration* (kg/m^3)
p = *Partial pressure* (N/m^2)
α = *Concentration exponent*
i = *Component index*
Π is the product operator.

The units of the reaction rate and the pre-exponential factor depend on the:

- Order of the reaction
- Concentration basis selected in the [Ci] Basis list box

The units for the pre-exponential factor are as follows:

When [Ci] Basis is	Units are: (To is not specified)	Units are: (To is specified)
Molarity	$\dfrac{\dfrac{kgmole-K^{-n}}{\sec-m^3}}{\left(\dfrac{kgmole}{m^3}\right)^{\Sigma\alpha_i}}$	$\dfrac{\dfrac{kgmole}{\sec-m^3}}{\left(\dfrac{kgmole}{m^3}\right)^{\Sigma\alpha_i}}$
Molality	$\dfrac{\dfrac{kgmole-K^{-n}}{\sec-m^3}}{\left(\dfrac{gmole}{kg\,H_2O}\right)^{\Sigma\alpha_i}}$	$\dfrac{\dfrac{kgmole}{\sec-m^3}}{\left(\dfrac{gmole}{kg\,H_2O}\right)^{\Sigma\alpha_i}}$
Mole fraction or Mass fraction	$\dfrac{kgmole-K^{-n}}{\sec-m^3}$	$\dfrac{kgmole}{\sec-m^3}$

Continued

When [Ci] Basis is	Units are: (To is not specified)	Units are: (To is specified)
Partial pressure	$\dfrac{\dfrac{kgmole-K^{-n}}{\sec-m^3}}{\left(\dfrac{N}{m^2}\right)^{\Sigma\alpha_i}}$	$\dfrac{\dfrac{kgmole}{\sec-m^3}}{\left(\dfrac{N}{m^2}\right)^{\Sigma\alpha_i}}$
Mass concentration	$\dfrac{\dfrac{kgmole-K^{-n}}{\sec-m^3}}{\left(\dfrac{kg}{m^3}\right)^{\Sigma\alpha_i}}$	$\dfrac{\dfrac{kgmole}{\sec-m^3}}{\left(\dfrac{kg}{m^3}\right)^{\Sigma\alpha_i}}$

Reactions With Solids

When modeling reactive systems containing solids, there are many ways to account for the effect of these solids in your simulation. Aspen Plus provides calculation options to appropriately model the effect of your solids on the reaction stoichiometry, the reaction rate, and volume basis for concentrations. The information in this section is designed to help you specify Reaction IDs that most accurately reflect your reactions.

Stoichiometry and Reaction Rate

When specifying a reaction on the Edit Reaction dialog box:

For Solids that	Specify
Participate in reactions and control the reaction rate.	Both stoichiometric coefficients and exponents.
Participate in reactions without controlling the reaction rate.	Only the stoichiometric coefficients for these solids, without entering exponents.
Act as catalysts by controlling reaction rates without participating in the reactions.	Only the exponents for these solids, without entering stoichiometric coefficients.
Are inert.	Neither stoichiometric coefficients nor exponents.

Volume Basis for Concentrations

When specifying information for the calculation of an equilibrium constant for equilibrium reactions, or a reaction rate for kinetic reactions, solid components can either be included or ignored in the denominator term of concentrations. To control how these calculations are performed, use the Solids button on Equilibrium sheet or the Kinetic sheet of your Reaction ID.

The Solids dialog box allows the following specifications with regard to the denominator term of component concentrations:

- For liquid and vapor component concentrations, you can include the reacting phase only, or the reacting phase and the solid phase, by clicking the appropriate option in the For Liquid or Vapor Component frame. The default is to include only the reacting phase.
- For solid component concentrations, you can include the solid phase only, or the solid and total liquid phases, by clicking the appropriate option in the For Solid Component frame. The default is to include only the solid phase.
- For wolid component concentrations, you can also include solid components in all substreams, or only those in the substream of the reacting solid, by click the appropriate option. The default is to include solids in all substreams.

Specifying LHHW Reactions for Reactors and Pressure Relief Systems

To specify Langmuir-Hinshelwood-Hougen-Watson (LHHW) kinetics for the reactor models RCSTR, RPlug, and RBatch, or for the pressure relief calculations in Pres-Relief, you need to:

- Define the type and stoichiometry of the reactions
- Enter equilibrium or kinetic parameters
- Specify optional adsorption expressions

To specify LHHW reactions:

1. From the Data menu, point to Reactions, then Reactions.
2. On the Reactions Object Manager, click New to create a new Reaction ID.
3. In the Create New ID dialog box, enter a reaction name in the Enter ID field, or accept the default ID.
4. Select LHHW in the Select Type list, and click OK.

Once the Reaction ID is created, you can begin defining reactions within the Reaction ID. There are two types of reactions allowed in a LHHW type Reaction ID.

Type	For
Equilibrium	Equilibrium reactions
Kinetic	Rate-controlled reactions

To specify the individual reactions within your LHHW Reaction ID, follow the instructions in subsequent sections of this chapter for the type of reaction you want to create.

Equilibrium Reactions for LHHW (for RCSTR only)

Specify equilibrium reactions for LHHW the same way as for Powerlaw reactions. See Specifying Power Law Reactions for Reactors and Pressure Relief Systems, this chapter.

Rate-Controlled Reactions for LHHW

For rate-controlled reactions, the LHHW rate expression can be written as:

$$\gamma = \frac{\text{(kinetic factor)(driving force expression)}}{\text{(adsorption expression)}}$$

Where:

Kinetic factor = $k\left(\frac{T}{To}\right)^n e^{(-E_a/R)[1/T-1/To]}$

Driving force expression = $K_1\left(\prod C_i^{v_i}\right)-K_2\left(\prod C_j^{v_j}\right)$

Adsorption expression = $\left\{\Sigma K_i\left(\prod C_j^{v_j}\right)\right\}^m$

Where:

r = Rate of reaction

k = Pre-exponential factor

T = Temperature in Kelvin

To = Reference temperature in Kelvin

n = Temperature exponent

E_a = Activation energy

R = Universal gas law constant

C = Component concentration

m = Adsorption expression exponent

K_1, K_2, K_i = Equilibrium constants

υ = Concentration exponent

i, j = Component index

Π is the product operator, and Σ is the summation operator.

The concentration terms C_i and C_j depend on the concentration basis you select:

$[C_i]$ basis	Concentration term C
Molarity	Component molar concentration (kgmole/m^3)
Molality	Component molality (gmole/kg H_2O)
Mole fraction	Component mole fraction
Mass fraction	Component mass fraction
Partial pressure	Component partial pressure (N/m^2)
Mass concentration	Component mass concentration (kg/m^3)

To add kinetic type reactions to your LHHW Reaction ID:

1. Click New on the Reactions Stoichiometry sheet of your LHHW Reaction ID.
2. On the Edit Reaction dialog box, Reaction Type defaults to Kinetic, and the reaction number is entered automatically. Enter components and stoichiometric coefficients to define the reaction. Coefficients should be negative for reactants and positive for products.
3. Click Close when finished. You should see your new reaction number, type, and equation displayed on the Stoichiometry sheet.

4. Repeat steps 1 through 3 for each additional kinetic reaction.
5. Select the Kinetic sheet.
6. On the Kinetic sheet, select a reaction from the list at the top of the sheet.
7. Specify in which phase the reaction will take place using the Reacting Phase list. The default is the liquid phase.
8. Enter the pre-exponential factor (k), the temperature exponent (n), and the activation energy (E) in the appropriate fields of the Kinetic Factor frame. The pre-exponential factor must be in the SI units described in Specifying Power Law Reactions for Reactors and Pressure Relief Systems, this chapter. The temperature exponent refers to temperature in Kelvin.
9. If solids are present, click the Solids button and select the appropriate options for calculation of concentration. For more information, see Reactions With Solids, this chapter.
10. Click the Driving Force button.
11. On the Driving Force Expression dialog box, select the concentration basis in the [Ci] Basis list. See Specifying Power Law Reactions for Reactors and Pressure Relief Systems, this chapter, for the definitions of the concentration basis options.
12. With the Enter Term value at the default of Term 1, enter the concentration exponents for reactants and products, and the coefficients for the driving force constant (A, B, C, and D) for term 1 of the driving force.
13. Select Term 2 in the Enter Term list.
14. Enter the concentration exponents for reactants and products, and the coefficients for the driving force constant (A, B, C, and D) for term 2 of the driving force expression.
15. Click Close when finished with both terms.
16. To specify optional adsorption expressions, click the Adsorption button.
17. On the Adsorption Expression dialog box, enter the overall exponent for the adsorption term in the Adsorption Expression Exponent field.
18. Specify concentration exponents by selecting components and entering an exponent for each term in the adsorption expression.
19. Specify adsorption constants by entering the Term No. and specifying the coefficients.

    The coefficients are for the following correlation:

    $$\ln K_i = A_i + B_i / T + C_i * \ln(T) + D_i * T$$

Where:

K_i = Equilibrium constant

T = Temperature in Kelvin

A_i, B_i, C_i, D_i = User-supplied coefficients

20. Repeat steps 6 through 19 for each additional LHHW kinetic reaction.

Specifying Reactions for Reactive Distillation

To specify reactions for reactive distillation in the distillation models, RadFrac, BatchFrac, and RateFrac, use the Reactions REAC-DIST forms to:

- Define reaction stoichiometry
- Enter equilibrium or kinetic parameters
- Specify parameters for user-defined kinetics

For RadFrac and RateFrac, you can also use the Reactions User forms to specify user-defined kinetics (see Using a User-Kinetics Subroutine, this chapter). The Reactions User forms is preferred because you can use the same user-defined kinetics in reactor or pressure relief calculations.

To create a new distillation reaction ID:

1. From the Data menu, point to Reactions then Reactions.
2. On the Reactions Object Manager, click New to create a new Reaction ID.
3. In the Create New ID dialog box, enter a reaction name in the Enter ID field, or accept the default ID.
4. Select REAC-DIST in the Select Type list, and click OK.

   Once the Reaction ID is created, you can begin defining reactions within the Reaction ID. There are four types of reactions allowed in a Reac-Dist Reaction ID.

Type	For
Equilibrium	Equilibrium reactions
Kinetic	Rate-controlled reaction
Conversion	Fractional conversion reaction (RadFrac only)
Salt	Electrolyte salt precipitation (RadFrac only)

5. To specify the individual reactions within your Reac-Dist reaction ID, follow the instructions in subsequent sections of this chapter for the type of reactions listed in the previous table.

Equilibrium Reactions

To add equilibrium type reactions to your Reaction ID:

1. Click New on the Reactions Stoichiometry sheet of your Reac-Dist Reaction ID.
2. In the Select Reaction Type dialog box, Kinetic/Equilibrium/Conversion is the default reaction type. Accept the default Reaction No. displayed or enter a new Reaction No. Click OK.
3. On the Edit Reaction dialog box, Reaction Type defaults to Equilibrium. Enter components and stoichiometric coefficients to define the reaction. Coefficients should be negative for reactants and positive for products. You should not specify exponents for equilibrium reactions.
4. Click Close when finished. You should see your new reaction number, type, and equation displayed on the Stoichiometry sheet.
5. Repeat steps 1 through 4 for each additional equilibrium reaction.
6. Click the Equilibrium sheet.
7. On the Equilibrium sheet, select a reaction from the list at the top of the sheet.
8. Specify the phase in which the reaction will occur in the Reacting Phase list. The default is the liquid phase.
9. Specify a calculation basis for the equilibrium constant by selecting an option in the Keq Basis list. The basis you choose defines how the equilibrium constant will be calculated, as discussed later in this section.
10. If the reaction does not actually reach equilibrium, you can specify Temperature Approach to Equilibrium. The temperature approach you enter will be added to the stage temperature to compute the equilibrium constant.

11. Choose whether you want to compute Keq from Gibbs energies or from a built in polynomial expression by selecting the appropriate radio button.

    If you choose Compute Keq From Gibbs Energies, you do not need to enter coefficients for the equilibrium constant. Aspen Plus will compute Keq from the reference state Gibbs free energy of the components. You can skip to step 12.

12. If you choose Compute Keq From Built-In Expression, you must enter coefficients for the built-in equilibrium constant expression:

    $$\ln Keq = A + B/T + C*\ln(T) + D*T$$

    Where:

    Keq = Equilibrium constant

    T = Temperature in Kelvin

    A, B, C, D = User-supplied coefficients

    The definition of *Keq* depends on the basis you select in the Keq Basis list box.

Kbasis	**Equilibrium Constant Definition**[†]
Mole gamma (default)	$K=\Pi (x_i \gamma_i)^{\upsilon_i}$ (liquid only)
Molal gamma	$K=\Pi (m_i \gamma_i)^{\upsilon_i}$ (electrolytes, liquid only)
Mole fraction	$K=\Pi (x_i)^{\upsilon_i}$
Mass fraction	$K=\Pi (x_i^m)^{\upsilon_i}$
Molarity	$K=\Pi (C_i)^{\upsilon_i}$
Molality	$K=\Pi (m_i)^{\upsilon_i}$ (liquid only)
Fugacity	$K=\Pi (f_i)^{\upsilon_i}$
Partial pressure	$K=\Pi (p_i)^{\upsilon_i}$ (vapor only)
Mass concentration	$K=\Pi (C_i^m)^{\upsilon_i}$

[†] Where:

K = Equilibrium constant
x = Component mole fraction
x^m = Component mass fraction
C = Molarity (kgmole/m^3)
m = Molality (gmole/kg-H_2O)
γ = Activity coefficient
f = Component fugacity (N/m^2)
p = Partial pressure (N/m^2)
C^m = Mass concentration (kg/m^3)
υ = Stoichiometric coefficient (positive for products, negative for reactants)
i = Component index
Π = Product operator

All properties refer to the phase selected in the Reacting Phase field.

13. Repeat steps 7 through 12 for each equilibrium reaction.

Rate Controlled Reactions

Reactive distillation kinetics can be represented with a built-in Power Law expression, or a user kinetics subroutine. The following procedure shows how to use either method.

To add kinetic type reactions to your Reaction ID:

1. Click New on the Reactions Stoichiometry sheet of your Reac-Dist Reaction ID.
2. In the Select Reaction Type dialog box, Kinetic/Equilibrium/Conversion is the default reaction type. Accept the default Reaction No. displayed or enter a new Reaction No. Click OK.
3. On the Edit Reaction dialog box, select Kinetic from the Reaction Type list.
4. Enter components and stoichiometric coefficients to define the reaction. Coefficients should be negative for reactants and positive for products.
5. Specify Power Law exponents for each component. These exponents represent the *order* of the reaction with respect to each component. If you wish to specify a user kinetics subroutine to compute the reaction rates, do not enter exponents on this sheet.
6. Click Close when finished. You should see your new reaction number, type, and equation displayed on the Stoichiometry sheet.
7. Repeat steps 1 through 6 for each additional kinetic reaction.
8. Select the Kinetic sheet.
9. On the Kinetic sheet, select the appropriate option to use the built-in Power Law expression, or a user kinetic subroutine to represent the kinetics for the current Reaction ID.

10. Select a reaction from the list and specify in which phase the reaction will take place using the Reacting Phase list. The default reacting phase is liquid.
11. To use a user kinetics subroutine, you do not need to enter any further information on this sheet. Select the Subroutine tab of the reaction form, and specify the subroutine name in the Name field.

    For RadFrac and RateFrac, you can also specify user-defined kinetics on the Reactions User forms (see Using a User-Kinetics Subroutine, this chapter). The Reactions User forms is preferred because you can use the same user-defined kinetics in reactor or pressure relief calculations. For more information on using and writing user kinetics models, see *Aspen Plus User Models*.

    The rest of this procedure assumes you are using the built in Power Law.
12. To use the built-in Power Law expression, enter the pre-exponential factor (k), the temperature exponent (n), and the activation energy (E) on the Kinetic sheet of the Reactions form. The pre-exponential factor must be in the SI units described later in this section. The temperature exponent refers to temperature in Kelvin.
13. In the [Ci] Basis list, select the concentration basis. The concentration basis determines which form of the power law expression will be used, as discussed later in this section.
14. Repeat steps 10 through 13 for each kinetic reaction.

The power law expression depends on the concentration basis you select in the [Ci] Basis list box:

[Ci] Basis	**Power Law Expression**[†] **(To is not specified)**	**Power Law Expression**[†] **(To is specified)**
Molarity (default)	$r = kT^n e^{-E/RT} \Pi (C_i)^{\alpha_i}$	$r = k (T/To)^n e^{(-E/R)[1/T-1/To]} \Pi (C_i)^{\alpha_i}$
Molality (electrolytes only)	$r = kT^n e^{-E/RT} \Pi (m_i)^{\alpha_i}$	$r = k (T/To)^n e^{(-E/R)[1/T-1/To]} \Pi (m_i)^{\alpha_i}$
Mole fraction	$r = kT^n e^{-E/RT} \Pi (x_i)^{\alpha_i}$	$r = k (T/To)^n e^{(-E/R)[1/T-1/To]} \Pi (x_i)^{\alpha_l}$
Mass fraction	$r = kT^n e^{-E/RT} \Pi (x_i^m)^{\alpha_i}$	$r = k (T/To)^n e^{(-E/R)[1/T-1/To]} \Pi (x_i^m)^{\alpha_l}$
Partial pressure (vapor only)	$r = kT^n e^{-E/RT} \Pi (p_i)^{\alpha_i}$	$r = k (T/To)^n e^{(-E/R)[1/T-1/To]} \Pi (p_i)^{\alpha_i}$
Mass concentration	$r = kT^n e^{-E/RT} \Pi (C_i^m)^{\alpha_i}$	$r = k (T/To)^n e^{(-E/R)[1/T-1/To]} \Pi (C_i^m)^{\alpha_l}$

[†] *Where:*

r = Rate of reaction
k = Pre-exponential factor
T = Temperature in degrees Kelvin
To = Reference temperature in degrees Kelvin
n = Temperature exponent
E = Activation energy
R = Universal gas law constant
x = Mole fraction
x^m = *Mass fraction*
C = Molarity (kgmole/m³)
m = Molality (gmole/kg-H_2O*)*
C^m = *Mass concentration (kg/*m^3*)*
p = Partial pressure (N/m^2*)*
α = *Concentration exponent*
i = Component index
Π is the product operator.

The units of the reaction rate and the pre-exponential factor depend on the:

- Order of the reaction
- Holdup basis used by the distillation block
- Concentration basis selected in the [Ci] Basis list box

The units for the pre-exponential factor are as follows:

When [Ci] Basis is	**Units are:** **(To is not specified)**	**Units are:** **(To is specified)**
Molarity	$\dfrac{\dfrac{kgmole - K^{-n}}{\sec - (holdup\ unit)}}{\left(\dfrac{kgmole}{m^3}\right)^{\Sigma\alpha_i}}$	$\dfrac{\dfrac{kgmole}{\sec - (holdup\ unit)}}{\left(\dfrac{kgmole}{m^3}\right)^{\Sigma\alpha_i}}$

Continued

When [Ci] Basis is	Units are: (To is not specified)	Units are: (To is specified)
Molality	$\dfrac{\dfrac{kgmole-K^{-n}}{\sec-(holdup\ unit)}}{\left(\dfrac{gmole}{kg\ H_2O}\right)^{\Sigma\alpha_i}}$	$\dfrac{\dfrac{kgmole}{\sec-(holdup\ unit)}}{\left(\dfrac{gmole}{kg\ H_2O}\right)^{\Sigma\alpha_i}}$
Mole fraction or Mass fraction	$\dfrac{kgmole-K^{-n}}{\sec-(holdup\ unit)}$	$\dfrac{kgmole}{\sec-(holdup\ unit)}$
Partial pressure	$\dfrac{\dfrac{kgmole-K^{-n}}{\sec-(holdup\ unit)}}{\left(\dfrac{N}{m^2}\right)^{\Sigma\alpha_i}}$	$\dfrac{\dfrac{kgmole}{\sec-(holdup\ unit)}}{\left(\dfrac{N}{m^2}\right)^{\Sigma\alpha_i}}$
Mass concentration	$\dfrac{\dfrac{kgmole-K^{-n}}{\sec-(holdup\ unit)}}{\left(\dfrac{kg}{m^3}\right)^{\Sigma\alpha_i}}$	$\dfrac{\dfrac{kgmole}{\sec-(holdup\ unit)}}{\left(\dfrac{kg}{m^3}\right)^{\Sigma\alpha_i}}$

Where holdup unit is	When this is specified in the distillation block that uses the reactions
kgmole	Mole holdup or residence time
kg	Mass holdup
m^3	Volume holdup

Fractional Conversion Reactions (for RadFrac only)

Another way to define reactions in a distillation column is to calculate a conversion based on a built-in, temperature-dependent correlation.

To add conversion type reactions to your Reac-Dist Reaction ID:

1. Click New on the Reactions Stoichiometry sheet of your Reac-Dist Reaction ID.

2. In the Select Reaction Type dialog box, Kinetic/Equilibrium/Conversion is the default reaction type. Accept the default Reaction No. displayed or enter a new Reaction No. Click OK.
3. On the Edit Reaction dialog box, select Conversion from the Reaction Type list.
4. Enter components and stoichiometric coefficients to define the reaction. Coefficients should be negative for reactants and positive for products. You should not specify exponents for conversion reactions.
5. Click Close when finished. You should see your new reaction number, type, and equation displayed on the Stoichiometry sheet.
6. Repeat steps 1 through 5 for each additional conversion reaction.
7. Select the Conversion sheet.
8. If you have multiple conversion reactions within your Reaction ID, specify whether you want the conversion reactions to be computed simultaneously, or in series. By default, conversion reactions are assumed to occur simultaneously. If you want the conversions to be calculated in series, check the Reactions Occur in Series box. You must specify the same type for all conversion reactions. Series reactions take place in the order they are entered.
9. Select a reaction from the list.
10. In the Conversion Expression frame, select the component on which you will base the conversion of the selected reaction, in the Key Component list. Conversion is defined as the fractional conversion of the key component.
11. Enter the coefficients (A, B, C and D) for the fractional conversion correlation:

    $$Conv = A + B / T + C*\ln(T) + D*T$$

    You can also enter the conversion on the RadFrac Reactions Conversion sheet, to override the value computed from the conversion correlation.

Salt Precipitation Reactions (for RadFrac only)

In addition to liquid and vapor phase reactions, you also can specify salt precipitation reactions. These reactions are liquid/solid phase equilibrium reactions, where the solid phase consists of a single salt.

To add salt precipitation type reactions to your Reac-Dist Reaction ID:

1. Click New on the Reactions Stoichiometry sheet of your Reac-Dist Reaction ID.
2. On the Select Reaction Type dialog box, select Salt Precipitation in the Choose Reaction Type frame.

3. Select the component name of the salt in the Precipitating Salt list, and click OK.
4. On the Edit Salt dialog box, enter components and stoichiometric coefficients for the salt dissociation products.
5. Click Close when finished. You should see the new reaction displayed on the Stoichiometry sheet referenced by the component name of the salt.
6. Repeat steps 1 through 5 for each additional salt precipitation reaction.
7. Select the Salt sheet.
8. On the Salt sheet, select a salt from the Salt list.
9. If the reaction does not actually reach equilibrium, you can specify the Temperature Approach to Equilibrium. The temperature approach you enter will be added to the stage temperature to compute the equilibrium constant.
10. Choose whether you want to compute the equilibrium constant (solubility product) from Gibbs energies or from a built in polynomial expression by selecting the appropriate radio button.

    If you choose Compute Keq From Gibbs Energies, you do not need to enter coefficients for the equilibrium constant. Aspen Plus will compute Keq from the reference state Gibbs free energies of the components.
11. If you choose Compute Keq From Built-In Expression, you need to enter coefficients for the built-in equilibrium constant expression, and choose a concentration basis for the equilibrium constant in the Keq Basis field.

    The expression and equilibrium constant definitions are the same as for fluid phase equilibrium reactions. For more information, see Equilibrium Reactions, this chapter.

If no rate-controlled or fractional conversion fluid-phase reactions are present, it is recommended that you specify salt precipitation reactions as electrolyte chemistry reactions. The advantages are that Electrolyte Chemistry:

- Can be generated automatically by the Electrolytes Wizard
- Accesses the Aspen Plus electrolytes reaction database for equilibrium constant data

See Specifying Electrolytes Chemistry, this chapter.

Using a User-Kinetics Subroutine

To use a user-supplied kinetics subroutine to calculate reaction rates, you need to specify the Fortran subroutine name. Use the Reactions User forms to specify user-defined kinetics for:

- Reactor models (RCSTR, RPlug, and RBatch)
- Distillation models (RadFrac and RateFrac)
- Pressure relief calculations in Pres-Relief

For RadFrac and RateFrac, you can also use the Reactions Reac-Dist forms to specify user-defined kinetics (see Specifying Reactions for Reactive Distillation, this chapter). You can define equilibrium reactions to be solved simultaneously with rate-controlled reactions. Only RCSTR, RadFrac and RateFrac can handle equilibrium reactions.

To specify a user Fortran subroutine for reaction rates:

1. From the Data menu, point to Reactions then Reactions.
2. On the Reactions Object Manager, click New to create a new Reaction ID.
3. In the Create New ID dialog box, enter a reaction name in the Enter ID field, or accept the default ID.
4. Select User in the Select Type list, and click OK.
5. On the Reactions Stoichiometry sheet click New.
6. On the Edit Reaction dialog box, the default reaction type is Kinetic, and the reaction number is entered automatically. Enter components and stoichiometric coefficients to define the reaction. Coefficients should be negative for reactants and positive for products.
7. Click Close when finished. You should see your new reaction displayed on the Stoichiometry sheet.
8. Repeat steps 7 through 9 for each additional user kinetic reaction.
9. Select the Kinetic sheet.
10. On the Kinetic sheet, select a reaction from the list and specify in which phase the reaction will take place using the Reacting Phase list. The default is the liquid phase.
11. If solids are present, click the Solids button and select the appropriate options for calculation of concentration. See Reactions With Solids, this chapter for details.
12. Select the Subroutine sheet.
13. On the Subroutine sheet, enter the name of the user subroutine, in the Name field. For more information on using and writing user kinetics models, see *Aspen Plus User Models*.

For any equilibrium reactions within a User type Reaction ID, specify them as you would for equilibrium reactions within a Powerlaw Reaction ID. For details, see Specifying Power Law Reactions for Reactors and Pressure Relief Systems, this chapter.

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28 Property Sets

This chapter describes:

- What is a property set?
- How to specify a new or existing property set
- How to specify user properties for use in property sets
- Examples

About Property Sets

A property set is a collection of thermodynamic, transport, and other properties that you can use in:

- Stream reports
- Physical property tables and Analysis
- Unit operation model heating/cooling curve reports
- Distillation column stage property reports and performance specifications
- Reactor profiles
- Design specifications and constraints
- Fortran and sensitivity blocks
- Optimization and Data-Fit blocks

Aspen Plus has several built-in property sets that are sufficient for many applications. The list of built-in property sets is determined by the Template you choose when creating a new run. For more information on Templates,see Chapter 2.

You can use a built-in property set and modify it to fit your needs, or you can create your own property sets. To see the built-in sets available or select one, use the drop-down list on any property set list box. The list prompts describe the contents of each built-in property set.

Defining a Property Set

To define a property set:

1. From the Data menu, click Properties.
2. Double-click on the Prop-Sets folder in the left pane of the Data Browser.
3. To create a new property set, click New. In the Create New ID dialog box, enter a new property set ID or accept the default ID, and click OK.
4. Once the new property set has been created, to modify it (or any existing property set), select the name from the Object Manager and click Edit.

On the Properties sheet of the Prop-Sets form, you can select properties from the drop-down list in the Physical Properties field. Choose one or more properties to be included in your property set. When you make a selection, a prompt appears for each property.

Tip Use the Search button to find the properties you want included in the property set. For information on using the search dialog box see Using the Search Dialog Box, this chapter.

5. Select one or more units for the property, using the Units fields.

   If you select multiple units the property is reported in each of the units selected.

6. On the Prop-Sets Qualifiers sheet, specify the following qualifiers for the properties to be calculated:

   - Phase (total mixture, total liquid, vapor, 1st or 2nd liquid, and solid)
   - Components
   - 2nd liquid key components (key component to identify the 2nd liquid phase)
   - Temperature
   - Pressure
   - Percent distilled(points on petroleum distillation curves)
   - Water basis (wet or dry)

   Some qualifiers, such as temperature and pressure are optional. For more information, see *Aspen Plus Physical Property Data*, Chapter 4.

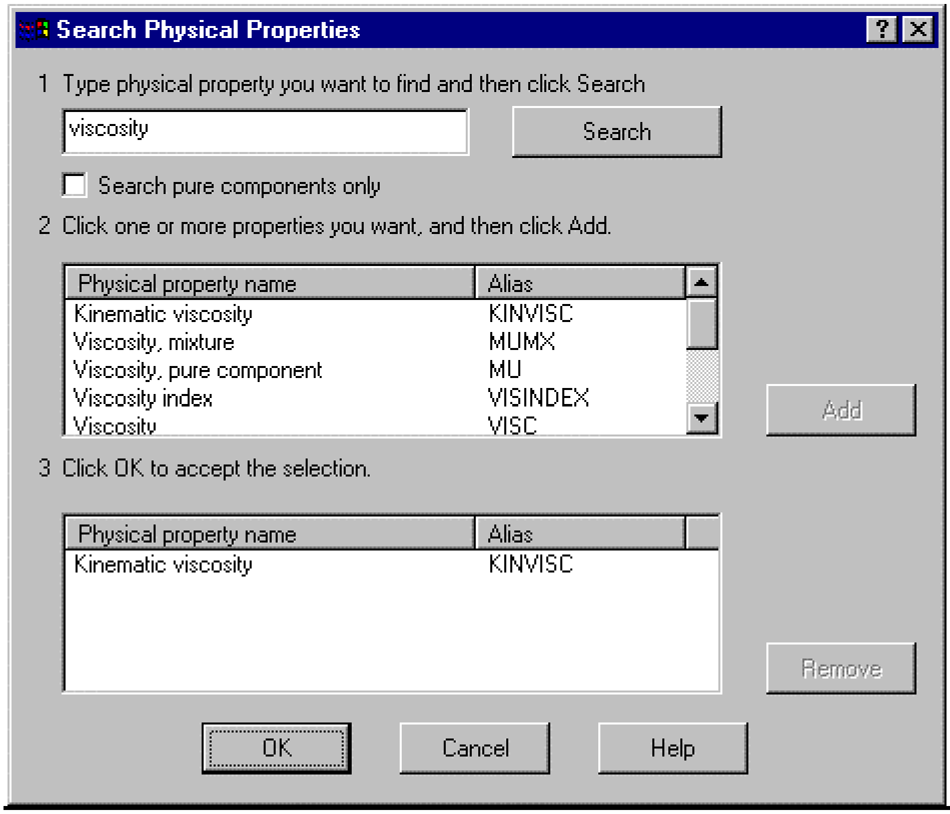
When you select multiple units and qualifiers, Aspen Plus computes the properties for each units specification and each valid combination of qualifiers.

Using the Search Dialog Box

If you want to search for a property by its common name, click the Search button on the Prop-Sets Properties sheet. A dialog box appears where you can type the name or a fragment of the name of the property you want. To add a property to your property set, select the property you desire and click Add. Once you have added all the properties you want, click OK to return to the Prop-Sets form.

Example of Using Search to Find Properties

Searching for the word “viscosity” shows a number of properties. Kinematic viscosity has been selected and added to the property set.



1 Type physical property you want to find and then click Search

viscosity

☐ Search pure components only

2 Click one or more properties you want, and then click Add.

Physical property name	Alias
Kinematic viscosity	KINVISC
Viscosity, mixture	MUMX
Viscosity, pure component	MU
Viscosity index	VISINDEX
Viscosity	VISC

3 Click OK to accept the selection.

Physical property name	Alias
Kinematic viscosity	KINVISC

Specifying Phase Qualifiers

The default for phase is Total. If a property cannot accept Total phase as a qualifier, you must enter an appropriate alternative (Liquid, Vapor, 1st liquid, 2nd liquid, or Solid).

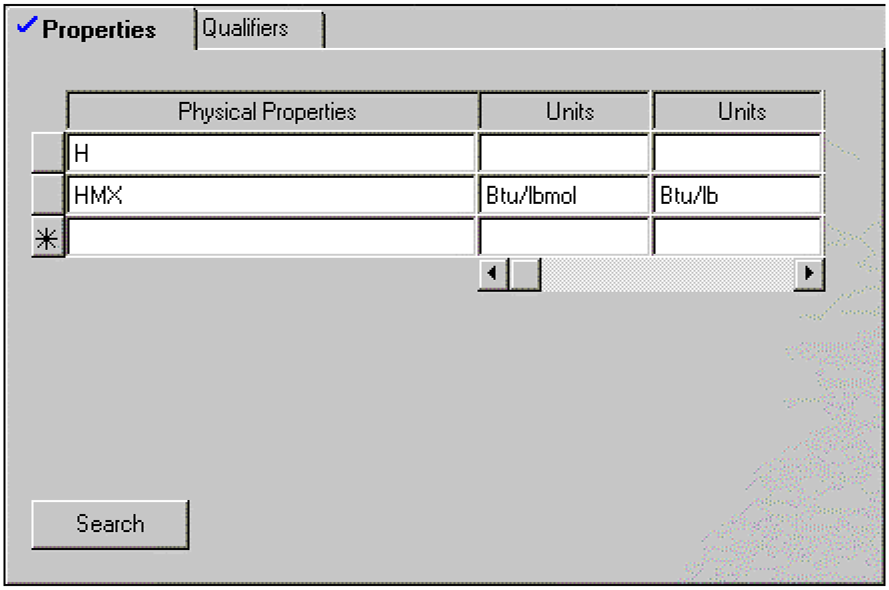
The phases you select should be consistent with the type of calculation desired. For example, if you request 1st and 2nd liquid phase properties for a heating/cooling curve for a Heater block, the block should perform either rigorous three-phase or free-water calculations.

Specifying Temperature and Pressure Qualifiers

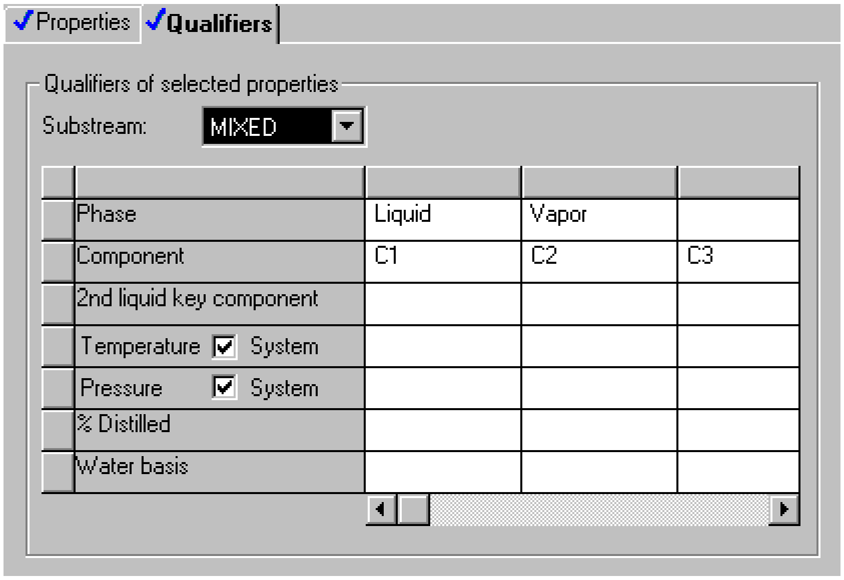
By default, Aspen Plus calculates properties at the stream conditions. Alternatively, you can specify the temperature and pressure for property calculations in the Temperature and Pressure fields of the Prop-Sets Qualifiers sheet. These specifications do not affect the composition of vapor and liquid phases, which are determined at the stream temperature and pressure.
Aspen Plus determines the units for the Temperature and Pressure specifications from the Units-Set you specify.

Example of Property Set for Reporting Enthalpy

Define a property set consisting of the pure component liquid and vapor enthalpies (H) of components C1, C2, and C3, as well as the mixture enthalpies (HMX) for the vapor and liquid phases. HMX is calculated on both a mole and mass basis.



Physical Properties	Units	Units
H		
HMX	Btu/lbmol	Btu/lb



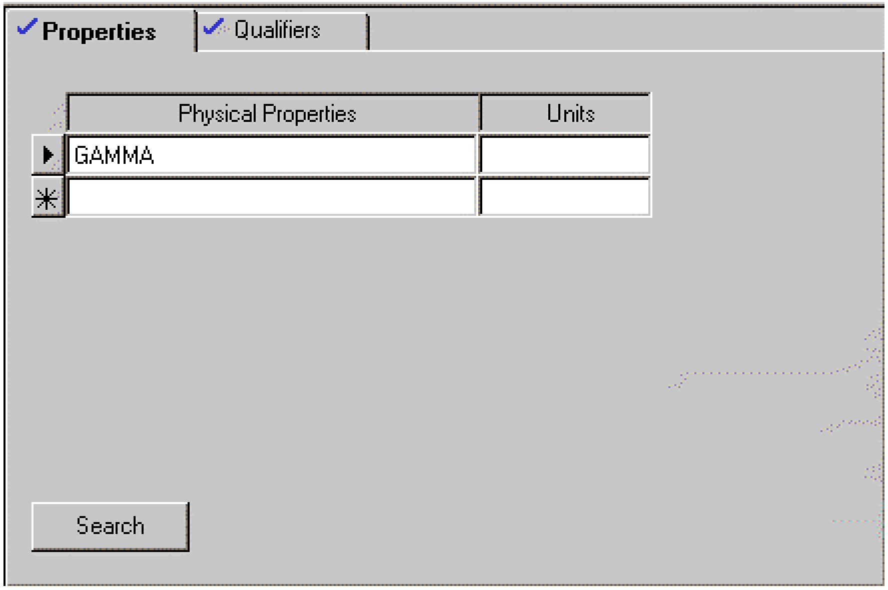
Qualifiers of selected properties

Substream: MIXED

Phase	Liquid	Vapor	
Component	C1	C2	C3
2nd liquid key component			
Temperature ☑ System			
Pressure ☑ System			
% Distilled			
Water basis			

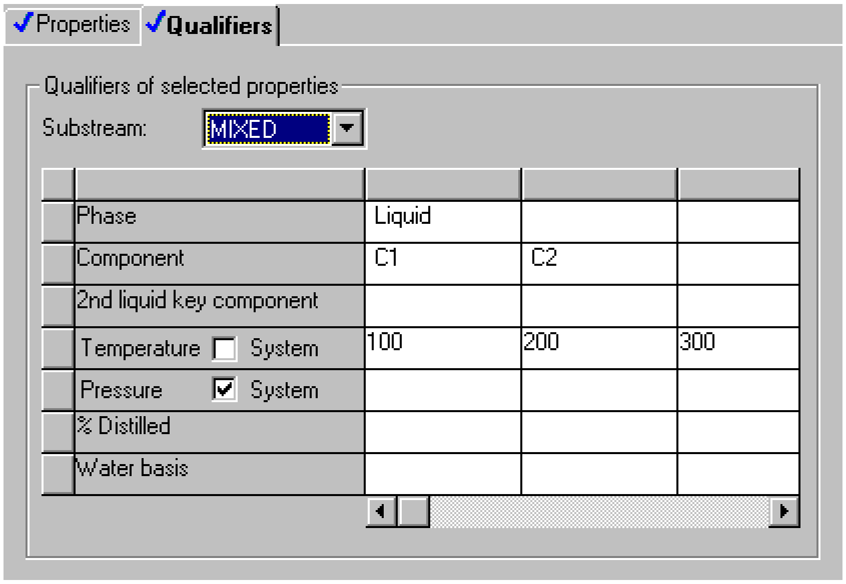
Example of Property Set for Activity Coefficients Over a Temperature Range

Define a property set consisting of the activity coefficients for components C1 and C2 in the liquid phase. The activity coefficients are evaluated at 100, 200, and 300°F.



Physical Properties	Units
GAMMA	

The units for the temperatures entered will be the temperature units of the ENG Units-Set, °F.



Qualifiers of selected properties

Substream: MIXED

Phase	Liquid		
Component	C1	C2	
2nd liquid key component			
Temperature ☐ System	100	200	300
Pressure ☑ System			
% Distilled			
Water basis			

User Defined Properties

You can define your own properties for use in property sets. You must supply a Fortran subroutine to calculate each property. See *Aspen Plus User Models* for more information about user subroutines.

To define an additional property for use in property sets:

1. From the Data menu, click Properties.
2. Open the Advanced folder by double-clicking on it in the left pane of the Data Browser.
3. Select UserProperties.
4. On the UserProperties Object Manager, click New.
5. Enter a user property ID or accept the default ID, and click OK
6. On the Specifications sheet, select whether your user property will be a standard property or an Assay curve property.
7. For standard properties, enter the name of the subroutine to be used for calculating the property, in the User Subroutine Name field.
8. Use the remaining fields on the Specifications sheet to enter information about the property.
9. On the Units sheet, specify whether you want any units conversion to be performed automatically by Aspen Plus, or within your user subroutine.

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29 Analyzing Properties

After you complete property specifications, you should analyze the properties predicted by your model to ensure correct results. You can do this using the Aspen Plus Property Analysis feature. Property Analysis generates tables of physical property values, which can be plotted to visualize and better understand the behavior of properties as predicted by your property specifications.

You can access Property Analysis via the following methods:

- Many commonly used tables and plots can be generated quickly and easily through an interactive method accessed from the Tools menu.
- Alternatively, generating Property Analyses from the Properties Analysis folder in the Data Browser Menu provides the most flexibility.

This chapter discusses each method of using the Property Analysis features and includes several examples.

Topics include:

- About Property Analysis
- Generating Property Analyses Interactively
  - Pure component properties
  - Properties for binary systems
  - Residue curves
  - Stream properties
- Generating Property Analyses Using Forms
  - Pure
  - Generic
  - Binary
  - PT-Envelopes
  - Residue curves
- Property Method Specifications for Property Analysis
- Examining Analysis Results

About Property Analysis

The Property Analysis feature generates tables of properties from variations in:

- Temperature
- Pressure
- Vapor fraction
- Heat duty
- Composition

The tables include property values that are defined using Property Sets, and can consist of thermodynamic, transport, and other derived properties. For more information on Property Sets and the properties they can include, see chapters 7 and 28.

You can use Property Analysis:

- On a standalone basis
- In a Flowsheet run
- In a Data Regression run

To use Property Analysis on a standalone basis, specify Property Analysis in the Run Type list on the Setup Specifications Global sheet. Or if you are creating a new run, specify Property Analysis in the Run Type list of the New dialog box.

Generating Property Analyses Interactively

This section describes how to generate many common analyses interactively, using the Analysis commands from the Tools menu.

This method automates many of the steps required to generate a Property Analysis, and defines built-in plots that provide quick and easy access to commonly used information.

If the information you require can be generated from the interactive Analysis commands, this is always quicker and easier than creating the Analysis using forms.

If you require property information that is not available from the interactive Analysis commands, you should create the Analysis manually using forms. See subsequent sections of this chapter for details on creating Analyses manually using forms.

You can use the interactive Analysis commands at any time after you complete the properties specifications.

The interactive Analysis commands can generate:

- Pure component properties
- Properties for binary systems
- Residue maps for ternary systems
- Stream properties. To generate stream properties, you must define at least one material stream.

Pure Component Properties

Use the interactive Analysis Pure commands to calculate and display pure component properties as a function of temperature to:

- Check pure component data and parameter values
- Compare properties for components that belong to the same family. Family plots can reveal incorrect trends.
- Determine whether the property is extrapolated correctly when temperatures are outside correlation limits

To generate pure component properties as a function of temperature, using the interactive Analysis Pure commands:

1. Ensure your Setup, Components, and Properties specifications are complete.
2. From the Tools menu, click Analysis, then Property, then Pure.

   On the Pure Component Properties Analysis dialog box, most of the required information is set to defaults, including:

Item	Information
Property Method	The global property method is used, as specified on the Properties Specifications Global sheet. You can select any Property Method that appears on the Properties Specifications form.
Temperature	The default is a temperature range from 0 to 25°C. You can enter a new range by modifying the lower and upper temperatures, or you can change from a temperature range to a temperature list, and specify a list of discreet temperature values.
Number of points to be tabulated	The default is 41 points. You can change the number of points, or enter a temperature increment.
Pressure	The default is 1 atm. You must change the default for vapor properties, for liquid properties near the critical point., and properties generated from EOS property methods.

3. From the Property list box, select the property to be tabulated.

   The Property list box displays the properties of the type shown in the Property Type list box.

   To focus your search for a property, you can change the property type to Thermodynamic or Transport. To see a list of all available properties, change the property type to All.

   This table shows the available thermodynamic properties:

Property	Property
Availability	Free energy
Constant pressure heat capacity	Enthalpy
Heat capacity ratio	Fugacity coefficient
Constant volume heat capacity	Fugacity coefficient pressure correction
Free energy departure	Vapor pressure†
Free energy departure pressure correction	Density
Enthalpy departure	Entropy
Enthalpy departure pressure correction	Volume
Enthalpy of vaporization†	Sonic velocity
Entropy departure	

† *Ideal and activity coefficient property methods only*

   This table shows the available transport properties:

Property	Property
Thermal conductivity	Surface tension
Viscosity	

   Optionally you can specify the units for the selected property in the Units list. If you do not specify the units, they will be determined by the output results Units-set specified on the Setup Specifications Global sheet.

4. Select the phase(s) for which you want the property to be reported, by clicking one or more of the Phase check boxes: Vapor, Liquid or Solid. Liquid is the default. Not all phases are valid for all properties. For a list of valid phases for each property, see *Aspen Plus Physical Property Data*, chapter 4.
5. Choose components by selecting one or more from the Available Components list, and clicking the right arrow button to move them to the Selected Components list.

6. When finished, click Go to generate the results.

   – or –

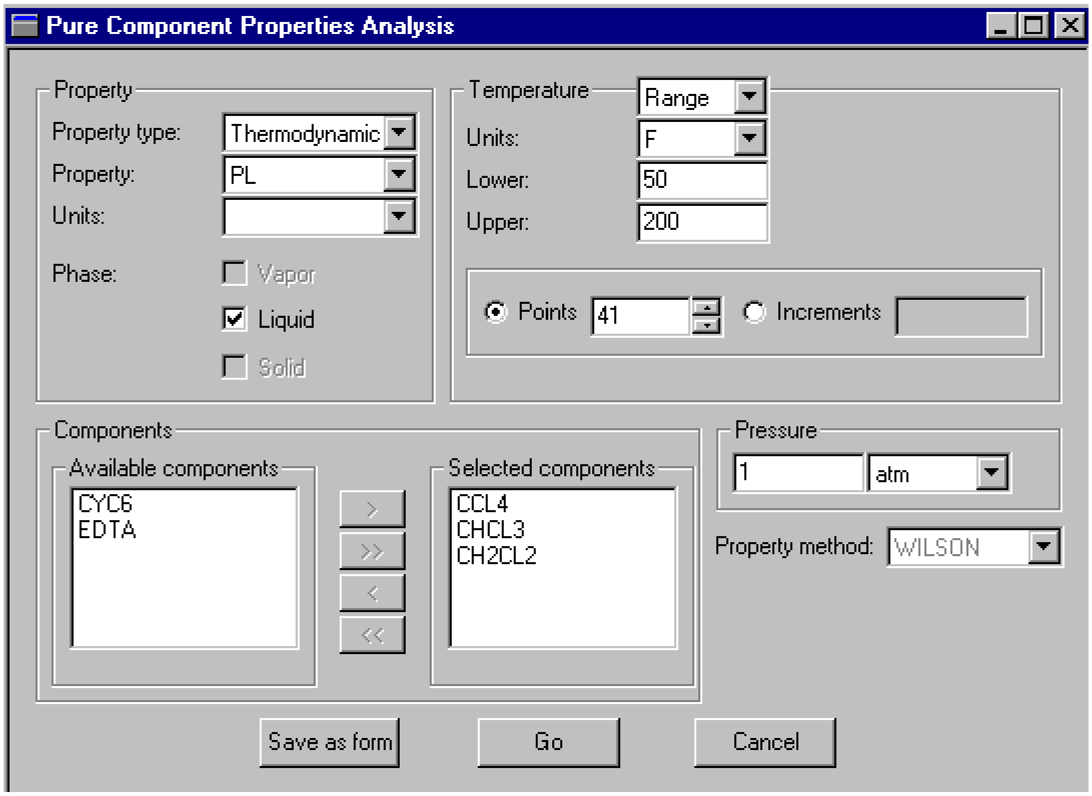
   Click Save As Form to save the interactive Property Analysis you have created to forms within the Properties Analysis section of the Data Browser menu. Saving an interactive Property Analysis as forms, allows you to preserve the input and results of this Property Analysis to view or modify at a later time. For more information on using forms to create Property Analyses, see Creating A Property Analysis, this chapter.

   Aspen Plus calculates the property at the temperature values you specify. Results appear in a form window and a plot. The plot displays results for all components you select.

Example of Examining Component Vapor Pressures

Calculate and display the vapor pressures of CCL_4, CH_2CL_2, and $CHCL_3$, between 50 and 200°F, using the IDEAL Property Method. To do this:

1. From the Tools menu, point to Analysis, then Property, then Pure.
2. The Pure Component Properties Analysis dialog box appears.



Property type: Thermodynamic
Property: PL
Units:
Phase: ☐ Vapor ☑ Liquid ☐ Solid

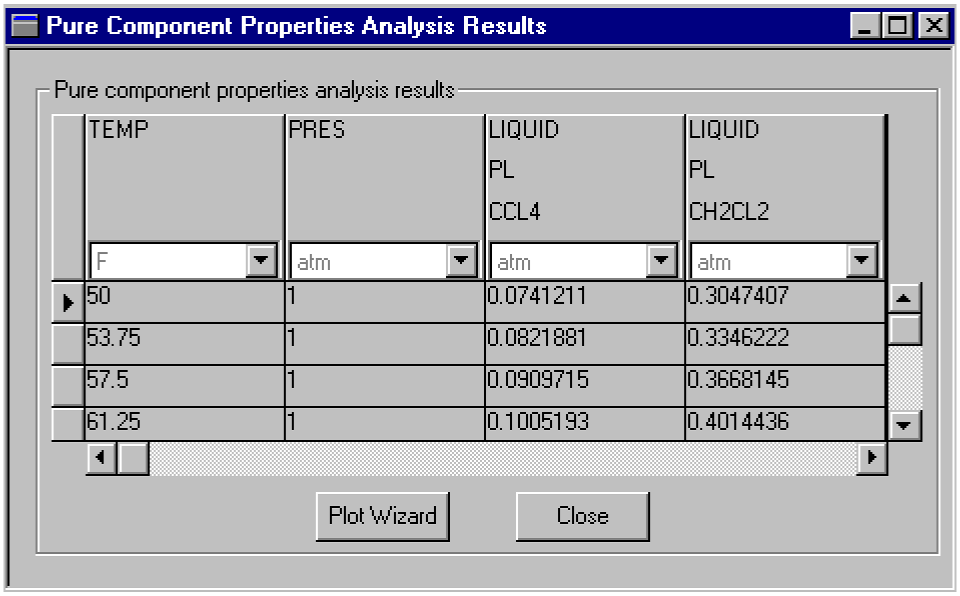
Temperature: Range
Units: F
Lower: 50
Upper: 200
● Points 41 ○ Increments

Available components: CYC6, EDTA
Selected components: CCL4, CHCL3, CH2CL2

Pressure: 1 atm
Property method: WILSON

3. When you have finished choosing your components, click Go to generate the results.

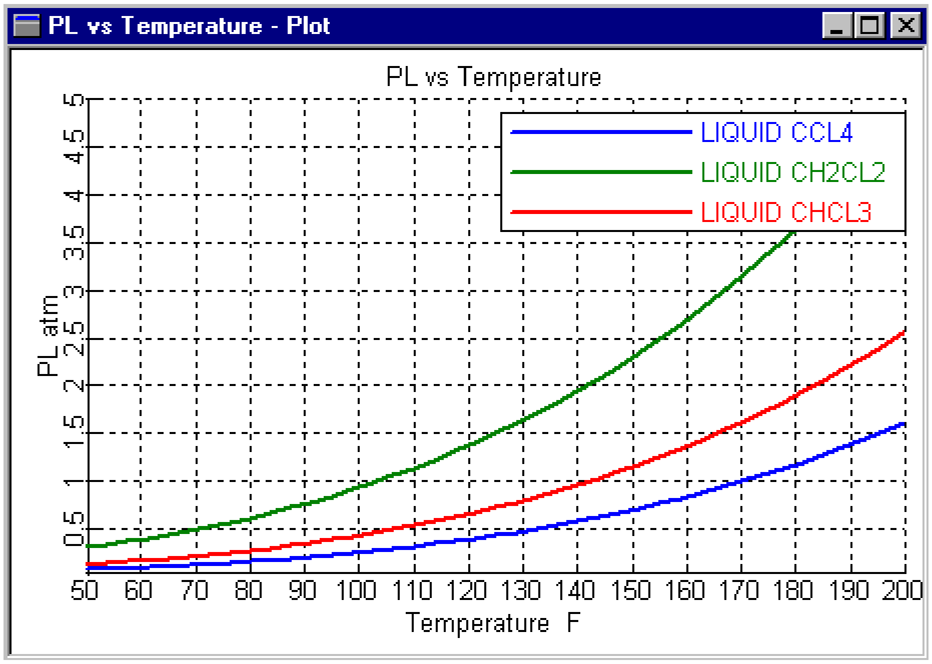
Tabular results form:



Pure component properties analysis results

TEMP	PRES	LIQUID PL CCL4	LIQUID PL CH2CL2
F	atm	atm	atm
50	1	0.0741211	0.3047407
53.75	1	0.0821881	0.3346222
57.5	1	0.0909715	0.3668145
61.25	1	0.1005193	0.4014436

Plotted results:



Properties for Binary Systems

You can generate common phase diagrams for binary systems to:

- Check the validity of data and parameter values
- Assess the degree of nonideality
- Check for existence of azeotropes
- Check for existence of two liquid phases
- Check quality of extrapolation of the model

To generate properties for binary systems use the Analysis Binary commands. To do this:

1. Ensure your Setup, Components, and Properties specifications are complete.
2. From the Tools menu, click Analysis, then Property, then Binary.
3. On the Binary Analysis dialog box, choose the type of Analysis in the Analysis Type list box:

Use analysis type	To tabulate
Txy	Temperature (T) versus liquid (x) and vapor (y) compositions at given pressures
Pxy	Pressure (P) versus liquid (x) and vapor (y) compositions at given temperatures
Gibbs energy of mixing	Gibbs energy of mixing versus liquid compositions at given temperatures and pressures. Used to detect the formation of two liquid phases.

For all three types of Binary Analysis, you can accept the default settings or specify the following information:

Item	Information
Components	Two are required. Use the Component 1 and Component 2 lists to choose the pair of components you wish to study. Only conventional components that are not solids or ions are allowed. Defaults are the first two conventional components listed on the Components Specifications Selection sheet.
Composition basis - Mole fraction or mass fraction	The default is mole fraction.
Composition component	This designates which component's composition is varied to generate the results. The default is the component selected as Component 1.

Continued

Item	Information
Composition - range or list	To determine at what compositions Aspen Plus will perform its calculations, you can specify a composition range or a composition list. The default is the full composition range between pure component 1 and pure component 2. You can either modify the default composition range, or change to a composition list, and specify a list of discreet compositions.
Number of points to generate	The default is 41 points. You can modify the number of points, or specify an increment of composition. Note that this only applies when using a composition range.
Property Method, Henry Components, Chemistry ID, and simulation approach	Defaults are obtained from the Properties Specifications Global sheet. For electrolyte systems, you should use the apparent components approach.

The remaining specifications for an interactive Binary Analysis depend on the Analysis type. The following sections provide instructions for specifying each type of Analysis.

Completing the Specifications for Txy Binary Analysis

To complete the specifications for a Txy type Binary Analysis, you can either modify the following specifications or accept the defaults.

For	You can specify	The default is
Valid Phases	Rigorous Vapor-Liquid, Vapor-Liquid-Liquid, or Vapor-Liquid-FreeWater calculations	Vapor-Liquid
Pressure(s)	You may specify a single pressure, or multiple pressures by entering a list of values, or by giving a range of values. If you choose to specify a range of values, you must enter number of points or an increment size.	A single pressure of 1 atm

When finished, you can simply click the Go button to generate the Txy diagram, or you can first click the Save As Form button to save the interactive Property Analysis you have created, to forms within the Properties Analysis section of the Data Browser menu.

Saving an interactive Property Analysis as forms allows you to preserve the input and results of this Property Analysis to view or modify at a later time. For more information on using forms to create Property Analyses, see Generating Property Analyses Using Forms, later this chapter.

Aspen Plus displays the results in tabular form in a form window and as a plot. If you specify more than one pressure, Txy diagrams for all the pressures appear on a single plot. In addition to the Txy diagram, you can display other plots from the Txy analysis results using the Plot Wizard. The following plots are available:

Type of Plot	Description
TXY	Temperature versus liquid and vapor composition
TX	Temperature versus liquid composition
YX	Vapor versus liquid composition
Gamma	Liquid activity coefficients of both components versus liquid composition
KVL	K-values of both components versus liquid composition

Displaying Txy Plots

To display these plots:

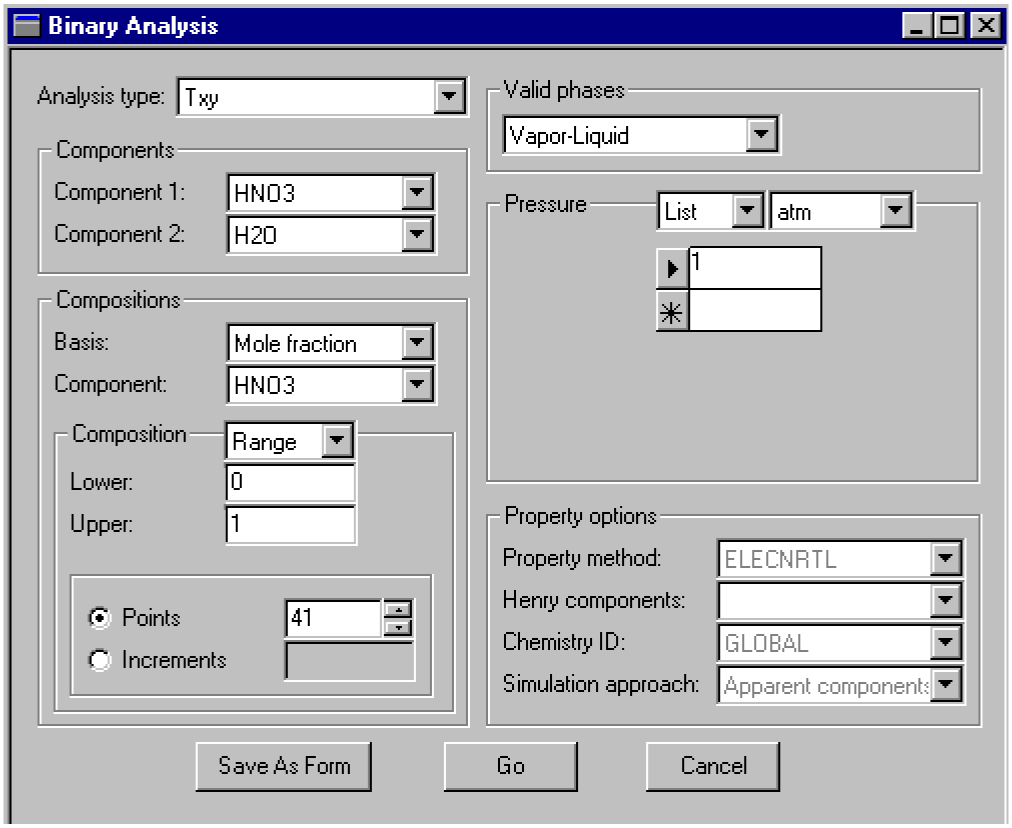
1. On the Binary Analysis Results window containing the tabular data, click the Plot Wizard button. The results window is behind the plot window.
2. On the Plot Wizard Step 1 window, click Next.
3. On the Plot Wizard Step 2 window, click the plot type you want.
4. To accept default plot settings, click Finish to generate the plot. Otherwise, click Next to enter additional settings and follow the remaining steps.
5. On the Plot Wizard Step 3 window, in the Component to Plot list box choose a component for which compositions will be displayed. If applicable, specify units for the plot variables.
6. Click Finish to accept defaults for the remaining plot settings and generate the plot.

   – or –

   Click Next to enter additional settings.
7. On the Plot Wizard Step 4 window, you can modify the defaults for plot title, axis titles, display options, grid or line type. You can also specify whether you want the plot to be automatically updated when new results are available.
8. Click Finish to generate the plot.

Example of Generating Txy Curves

Generate Txy curves at 1 atm and 2 atm for a mixture of HNO_3 and water, using the ELECNRTL property method and GLOBAL solution chemistry.



Binary Analysis

Analysis type: Txy

Components

Component 1: HNO3

Component 2: H2O

Compositions

Basis: Mole fraction

Component: HNO3

Composition: Range

Lower: 0

Upper: 1

● Points 41

○ Increments

Valid phases: Vapor-Liquid

Pressure: List atm

1

Property options

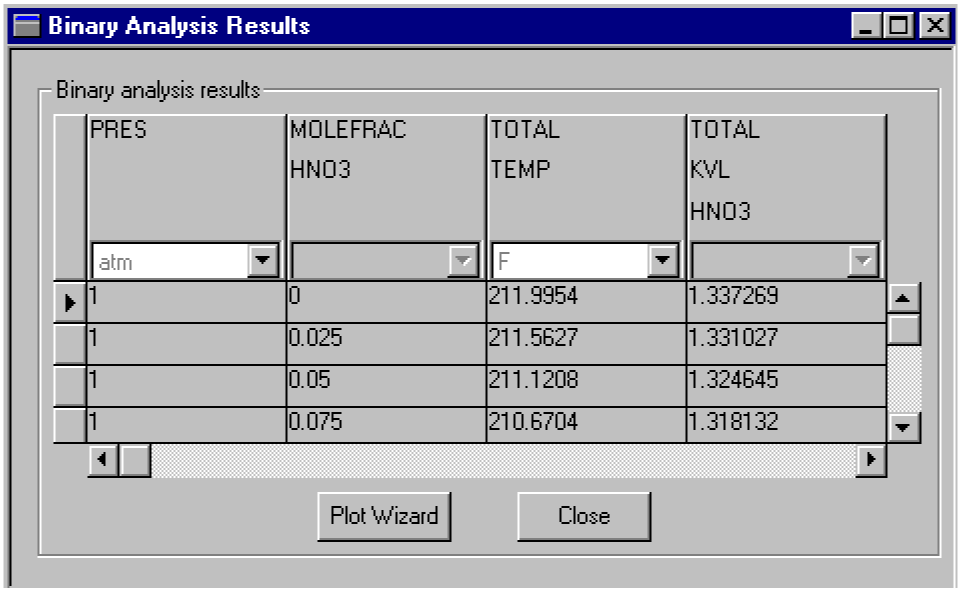
Property method: ELECNRTL

Henry components:

Chemistry ID: GLOBAL

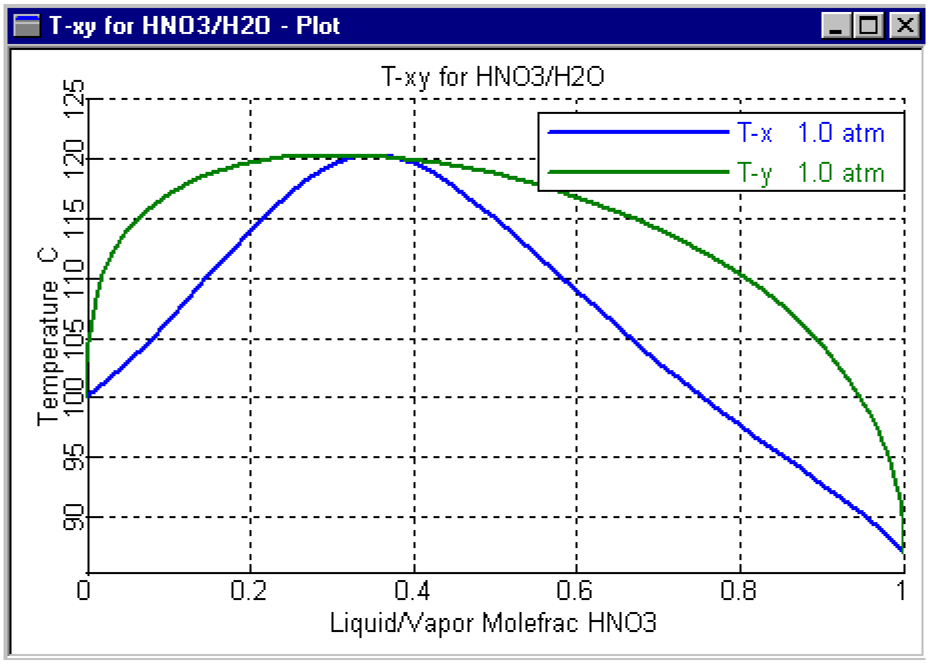
Simulation approach: Apparent components

Tabular results form:



PRES	MOLEFRAC HNO3	TOTAL TEMP	TOTAL KVL HNO3
atm		F	
1	0	211.9954	1.337269
1	0.025	211.5627	1.331027
1	0.05	211.1208	1.324645
1	0.075	210.6704	1.318132

Plotted results:



Completing the Specifications for Pxy Binary Analysis

To complete the specifications for a Pxy type Binary Analysis, you can either modify the following specifications or accept the defaults:

For	You can specify	The default is
Valid Phases	Rigorous Vapor-Liquid, Vapor-Liquid-Liquid, or Vapor-Liquid-FreeWater calculations	Vapor-Liquid
Temperature(s)	More than one temperature by entering a list of values, or by giving a range of values. If you choose to specify a range of values, you must enter number of points or an increment size.	A single temperature of 25°C

When finished, click Go to generate the Pxy diagram, or click Save As Form to save the interactive Property Analysis to forms within the Data Browser.

Saving an interactive Property Analysis as forms enables you to preserve the input and results of this Property Analysis to view or modify at a later time.

For more information on using forms to create Property Analyses, see Generating Property Analyses Using Forms, this chapter.

Aspen Plus displays the results in tabular form in a form window and as a plot. If you specify more than one temperature, Pxy diagrams for all the temperatures appear on a single plot.

In addition to the Pxy diagram, you can display other plots from the Pxy analysis results using the Plot Wizard. The following plots are available:

Type of Plot	Description
PXY	Pressure versus liquid and vapor composition
PX	Pressure versus liquid composition
YX	Vapor versus liquid composition
Gamma	Liquid activity coefficients of both components versus liquid composition
KVL	K-values of both components versus liquid composition

Displaying Pxy Plots

To display Pxy plots:

1. On the Binary Analysis Results window containing the tabular data, click the Plot Wizard button. The results window is behind the plot window.
2. On the Plot Wizard Step 1 window, click Next.
3. On the Plot Wizard Step 2 window, click the plot type you want.
4. To accept default plot settings, click Finish to generate the plot. Otherwise, click Next to enter additional settings.
5. On the Plot Wizard window, in the Component to Plot list box choose a component for which compositions will be displayed. If applicable, specify units for the resulting plot.
6. Click Finish to accept defaults for the remaining plot settings and generate the plot.

   – or –

   Click Next to enter additional settings.
7. On the Plot Wizard Step 4 window, you can modify the defaults for plot title, axis titles, display options, grid type or marker size. You can also specify whether you want the plot to be automatically updated when new results are available.
8. Click Finish to generate the plot.

Completing the Specifications for Gibbs Energy of Mixing

To complete the specifications for a Gibbs Energy of Mixing type Binary Analysis, you can either modify the following specifications or accept the defaults.

Item	Information
Units of Gibbs energy	If you do not specify the units, they will be determined by the Units-set specified on the Setup Specifications Global sheet.
Pressure	The default is 1 atm
Temperature(s)	The default is 25°C. You can specify more than one temperature, by entering a list of temperatures, or you can specify a range of temperatures and a number of points or an increment size.

When finished, click Go to generate the Gibbs energy of mixing versus x diagram, or click Save As Form to save your interactive Property Analysis to forms within the Data Browser.

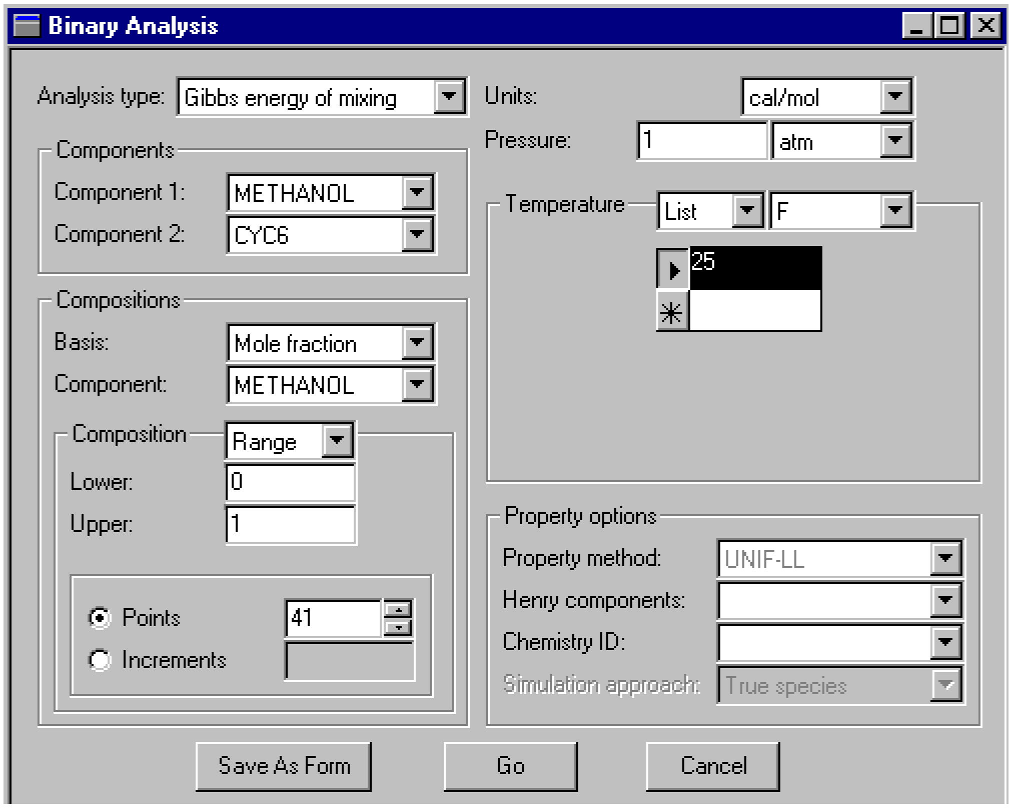
Saving an interactive Property Analysis as forms enables you to preserve the input and results of this Property Analysis to view or modify at a later time.

For more information on using forms to create Property Analyses, see Generating Property Analyses Using Forms, this chapter.

Aspen Plus displays the results in tabular form in a form window and as a plot. If you specify more than one temperature, Gibbs energy of mixing diagrams for all the temperatures appear on a single plot.

Example of Generating Gibbs Energy of Mixing

Generate a Gibbs Energy of Mixing diagram for methanol-cyclohexane at 25°C, using the UNIF-LL property method.



Analysis type: Gibbs energy of mixing

Units: cal/mol

Pressure: 1 atm

Components

Component 1: METHANOL

Component 2: CYC6

Temperature List F

25

Compositions

Basis: Mole fraction

Component: METHANOL

Composition Range

Lower: 0

Upper: 1

● Points 41

○ Increments

Property options

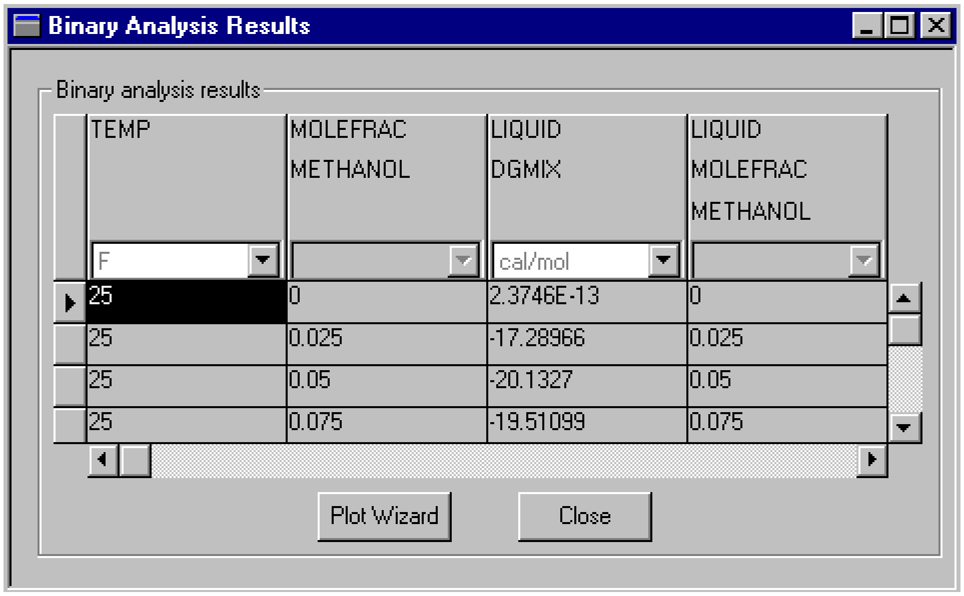
Property method: UNIF-LL

Henry components:

Chemistry ID:

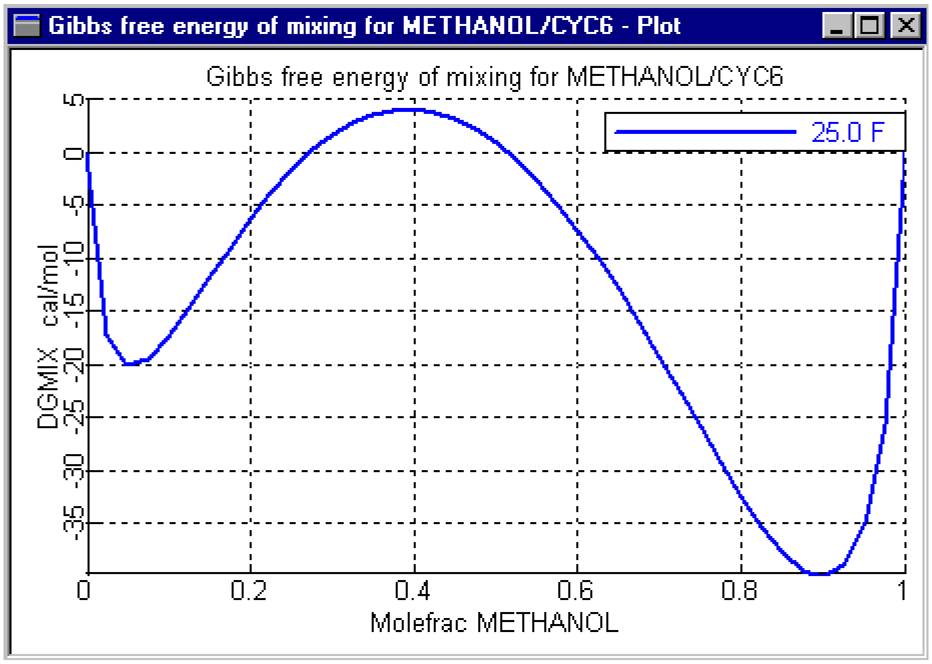
Simulation approach: True species

Tabular results form:



TEMP	MOLEFRAC METHANOL	LIQUID DGMIX	LIQUID MOLEFRAC METHANOL
F		cal/mol	
25	0	2.3746E-13	0
25	0.025	-17.28966	0.025
25	0.05	-20.1327	0.05
25	0.075	-19.51099	0.075

Plotted results:



Residue Curves

Residue Curves (or maps) plot the composition trajectories of a ternary mixture undergoing distillation at total reflux. You can use them to visualize the presence of azeotropes and the constraints azeotropes impose on the degree of separation.

Use Residue Curves to predict feasible splits, select entrainers, and analyze potential column operability problems.

Use Residue Curves with nonideal chemical systems, and property methods that represent such systems. Examples are activity-coefficient-based property methods, such as NRTL, Wilson, UNIQUAC, and UNIFAC. Do not use electrolyte property methods.

Generating Residue Curves

To generate Residue Curves using the interactive Analysis Residue commands:

1. Make sure your Setup, Components, and Properties specifications are complete.
2. From the Tools menu, point to Analysis, then Property, then Residue.
3. On the Residue Curves dialog box, Aspen Plus fills in defaults for all the required information. You can accept the defaults, or make changes to any of the following information:

Item	Information
Components	Three are required. Use the Component 1, Component 2, and Component 3 lists to choose the three components you wish to study. Only conventional components that are not solids or ions are allowed. Defaults are the first three conventional components listed on the Components Specifications Selection sheet.
Pressure	The default is 1 atm
Valid Phases	You can specify rigorous two phase (Vapor-Liquid) or three phase (Vapor-Liquid-Liquid) calculations. The default is Vapor-Liquid.
Number of curves	You can select 3-5 Curves, 10-15 Curves, or 15-20 Curves.
Property options	Defaults are obtained from the Properties Specifications Global sheet. For electrolyte systems, Aspen Plus uses the apparent components approach.

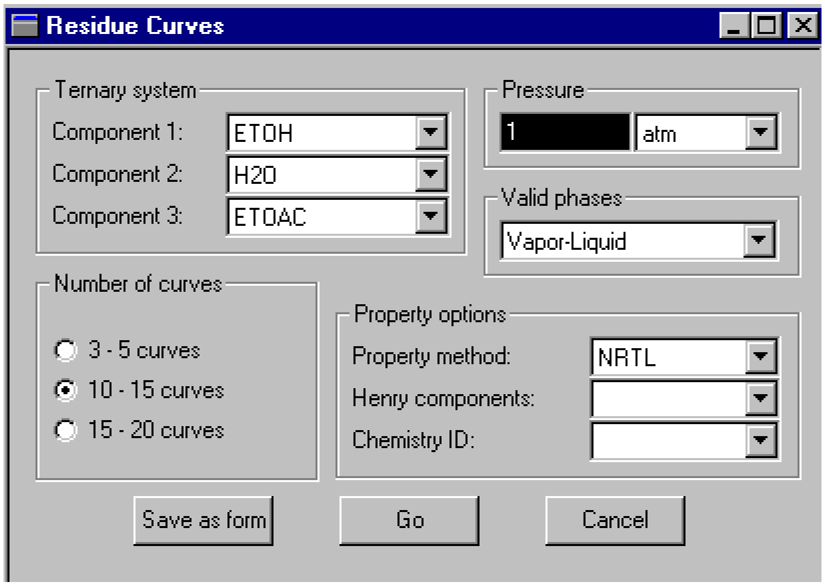
4. When finished, click Go to generate the residue curves, or first click the Save As Form button to save your interactive Property Analysis to forms within the Data Browser.

   Saving an interactive Property Analysis as forms enables you to preserve the input and results of this Property Analysis to view or modify at a later time.

Aspen Plus displays the results in tabular form, in a form window and as a triangular plot.

Example of Generating a Residue Map

Generate a residue map for the ternary system ethanol-water-ethyl acetate, at 1 atm, using the NRTL property method.



Residue Curves

Ternary system
Component 1: ETOH
Component 2: H2O
Component 3: ETOAC

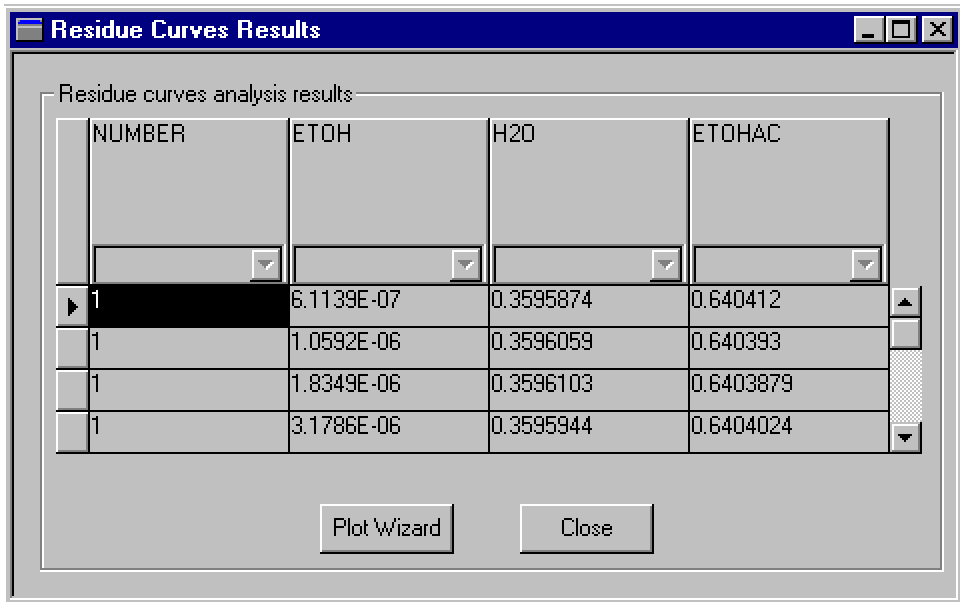
Pressure: 1 atm

Valid phases: Vapor-Liquid

Number of curves
○ 3 - 5 curves
● 10 - 15 curves
○ 15 - 20 curves

Property options
Property method: NRTL
Henry components:
Chemistry ID:

Tabular results form:

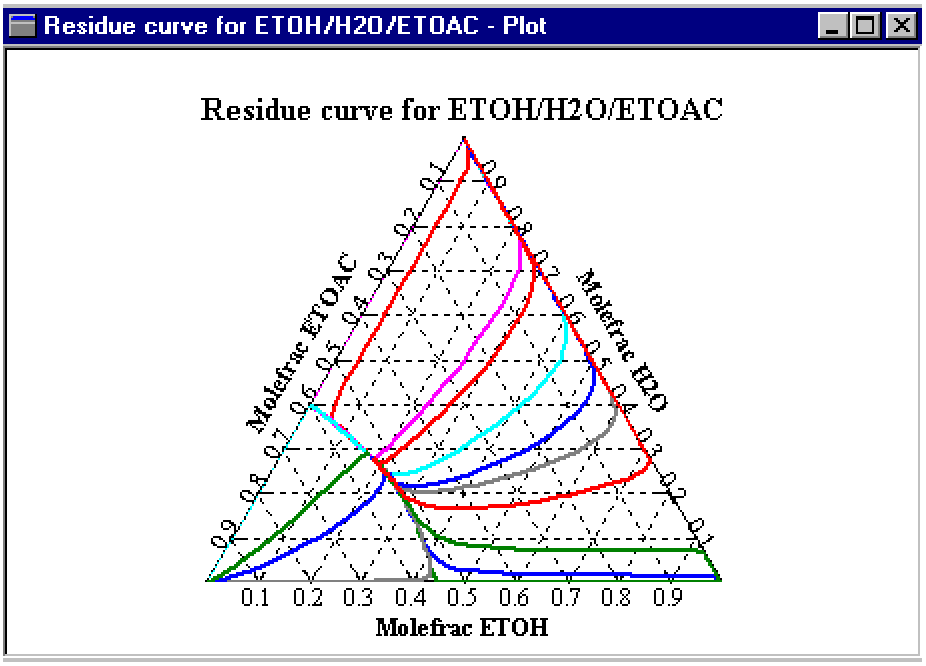


Residue Curves Results

Residue curves analysis results

NUMBER	ETOH	H2O	ETOHAC
1	6.1139E-07	0.3595874	0.640412
1	1.0592E-06	0.3596059	0.640393
1	1.8349E-06	0.3596103	0.6403879
1	3.1786E-06	0.3595944	0.6404024

Plotted results:



Stream Properties

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, to check your Property Method, you can analyze a feed stream as soon as you define it. 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 analyses 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 rates, and many thermodynamic and transport properties.
Component Flow	Component flow rates for the total stream and each of the phases present. Mole, mass, and standard liquid volume fractions are available.

Continued

Type	Description
Composition	Component fractions for the total stream and each of the phases present. Mole, mass, and standard liquid 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 Pressure-Temperature Envelopes, this chapter)

† *Plots can be generated from this analysis.*

†† *These analyses automatically display plots of the curves.*

Calculating and Displaying Stream Properties

To calculate and display stream properties interactively:

1. Ensure that Setup, Components, and Physical Properties specifications are complete.
2. Ensure the Stream Specifications sheet for the stream is complete or the stream has results that were calculated in the current session.
3. Click the stream on the flowsheet diagram to select it.
4. From the Tools menu, point to Analysis, then Stream, then the type of stream analysis you want to perform. The Stream Analysis types will be inactive if the conditions in steps 1,2 and 3 are not satisfied.
5. Make any selections and specifications in the dialog box for selecting options, and click OK. Each stream analysis type has defaults for required input, except temperature range for TV curves.

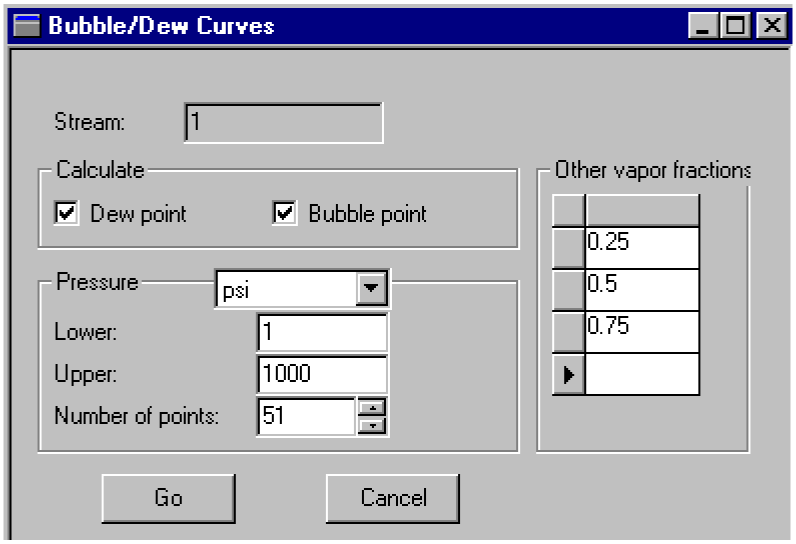
Stream analysis results appear in a form window. For some analysis types, a plot of the results also appears. Print or view these results and plots as you would with simulation results.

With the exception of the PT-Envelope type stream analysis, when you close the resulting forms and plots, ***the results are not saved.*** On the Ptenvelope dialog box, you are given the option to Save as Form, which will save the stream Property Analysis you have created interactively, to forms within the Properties Analysis section of the Data Browser menu. In all other types of stream analysis, you must redo the calculations if you want to look at them again, once you close the results forms.

Saving an interactive Property Analysis as forms allows you to preserve the input and results of this Property Analysis to view or modify at a later time. For more information on using forms to create Property Analyses, see Generating Property Analyses Using Forms, this chapter.

Example of Generating a Bubble/Dew Point Curve From Stream Analysis

The screens below show an example for generating a Bubble/Dew type stream analysis for a stream containing an equimolar mixture of ethane and n-heptane. The PENG-ROB property method is used.



Stream: 1

Calculate

☑ Dew point ☑ Bubble point

Pressure psi

Lower: 1

Upper: 1000

Number of points: 51

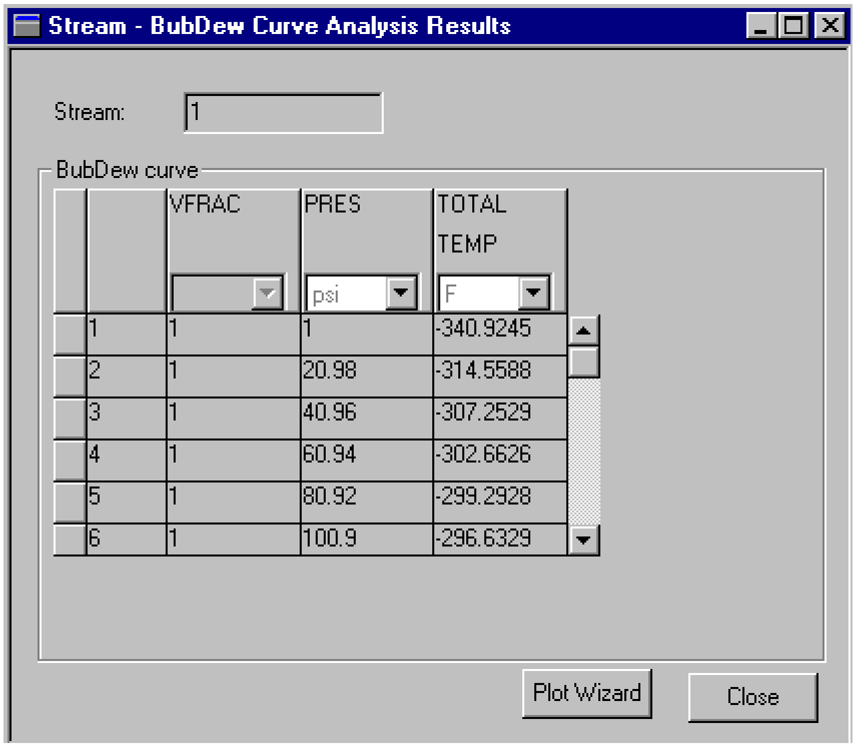
Other vapor fractions

0.25

0.5

0.75

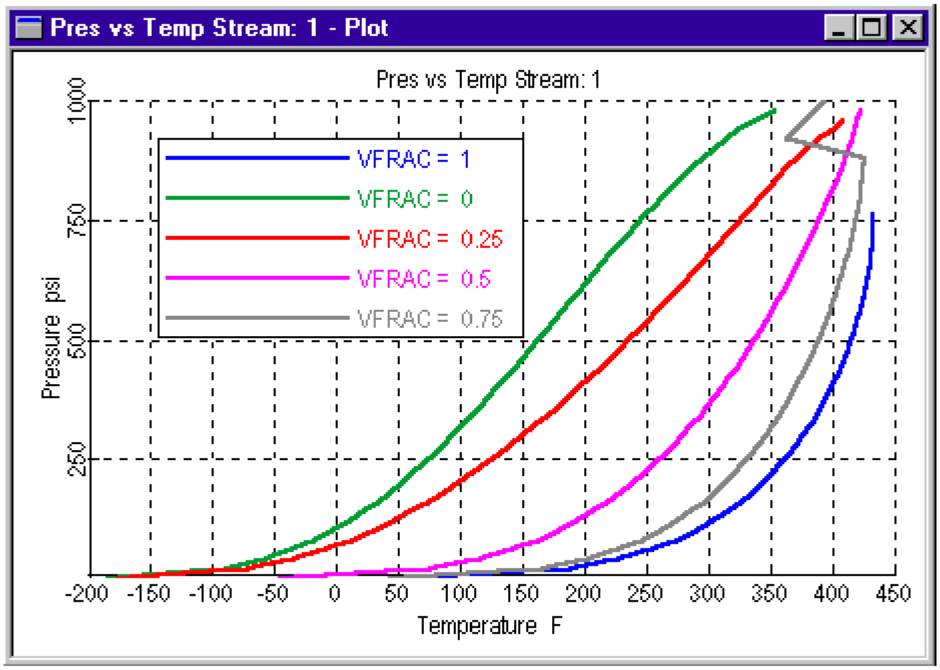
Tabular results form:



Stream: 1

	VFRAC	PRES psi	TOTAL TEMP F
1	1	1	-340.9245
2	1	20.98	-314.5588
3	1	40.96	-307.2529
4	1	60.94	-302.6626
5	1	80.92	-299.2928
6	1	100.9	-296.6329

Plotted results:



Generating Property Analyses Using Forms

In addition to the many tables and plots available through interactive Property Analysis, generating Property Analyses using forms provides the most flexibility because it:

- Generates tables of physical property values using specifications you enter on the Properties Analysis forms
- Allows you to report and study any property that you define in Property Sets

In general, you should only use manual Property Analysis when you need functionality that is not available within the simpler interactive Analysis commands.

The following Property Analyses types are available using forms:

Property Analysis Type	**For**
Pure †	Evaluation of pure component properties as a function of temperature and pressure
Binary †	Generating common phase diagrams for binary systems, such as Txy, Pxy, or Gibbs energy of mixing curves
Generic	Property evaluations for multi-phase mixtures from flash calculations, or single-phase mixtures without flash calculations
PT-Envelope	Pressure-temperature envelopes and properties along a constant vapor fraction line
Residue	Generating residue curve maps which plot the composition trajectories of a ternary mixture undergoing distillation at total reflux

† *You cannot create these analysis types using forms. You must use the interactive Analysis commands for these analysis types because the appropriate property sets are defined automatically. You can modify these analysis types using forms, but you should not modify the prop-sets created by the interactive Analysis because the Plot Wizard may not produce the correct plots. .*

Unlike the interactive method for using Property Analysis, when generating Analyses from forms, you must run the simulation to generate results. You can run the Property Analyses:

- On a standalone basis (Property Analysis run type)
- In a Flowsheet run
- In a Data Regression run

To use Property Analysis on a standalone basis, specify Property Analysis in the Run Type list on the Setup Specifications Global sheet (or the New dialog box when creating a new run).

Creating A Property Analysis Using Forms

To manually create a Property Analysis using forms:

1. Make sure your Setup, Components, and Properties specifications are complete.
2. From the Data menu, click Properties.
3. From the left pane of the Data Browser menu, click the Analysis folder.
4. On the Properties Analysis Object Manager, click New.
5. On the Create New ID dialog box, select the type of Analysis you want to create in the Select Type list.
6. Enter an ID for the new Analysis, or accept the default ID.
7. Click OK.

   The remaining specifications for using forms to generate a Property Analysis depend on the Analysis type. The following sections provide instructions for specifying each type of Analysis.

Pure

You must use the interactive Analysis commands to define your analysis, save the specifications as forms using the Save As Form button, then edit the form to add additional specifications. Use forms to modify pure component Property Analyses only when you need flexibility not afforded by the simpler interactive Analysis commands (for example results at multiple pressures).

Binary

You must use the interactive Analysis commands to define your analysis, save the specifications as forms using the Save As Form button, then edit the form to add additional specifications.

Generic

Use the Property Analysis Generic form to generate tables of properties of either:

- Multi-phase mixtures (for example, vapor and liquid) resulting from flash calculations
- Single-phase mixtures without flash calculations

The generic type of Property Analysis is the most flexible.

To generate a generic Property Analysis using forms:

1. On the System sheet of the Properties Analysis Generic Input form, click one of the options in the Generate frame to specify whether you want to generate properties at points along a flash curve for a multi-phase mixture resulting from flash calculations, or at points for single-phase mixtures without flash calculations.

   Click either Points Along a Flash Curve or Point(s) Without Flash.
2. In the System section, choose either to Specify Component Flow or Reference Flowsheet Stream. If you choose to specify component flow, enter the flowrates of your system. If you choose to reference a flowsheet stream, enter the Stream ID.
3. If you choose to specify component flow when generating points along a flash curve, specify the valid phases for flash calculations in the Valid Phases list. Choices are Vapor-Liquid, Vapor-Liquid-Liquid, or Vapor-Liquid-FreeWater. The default is Vapor-Liquid.
4. If you choose to reference a flowsheet stream when generating points along a flash curve, you can optionally specify the type of flash for the flowsheet stream, in the Flash Type list (see Notes in step 6.)
5. Click the Variable sheet.
6. On the Variable sheet, specify the Adjusted Variables and their values to be used in calculations.

   Notes:

   If a stream is referenced on the System sheet, you must either:

   - Vary two of temperature, pressure, vapor fraction, and duty
     – or –
   - Specify Flash Type on the System sheet

   If Flash Type is specified, any varied state variable must be consistent with that specification. Unspecified state variables default to the stream values. The number of valid phases is determined by the type of calculation performed to generate the referenced stream.

   If a stream is not referenced, you must either vary or specify on this form two of temperature, pressure, and vapor fraction.

You can define values for a varied variable by specifying either:

- A list of values
  – or –
- Upper and lower limits for the variable and either the number of points or the increment size.

7. Click the Tabulate sheet.

   On the Tabulate sheet, specify the Property Set(s) that contain properties you want to tabulate. To add a Property Set to the Selected Prop-Sets list, select it from the Available Prop-Sets list, and click the right arrow button. To select all available Property Sets, click the double right arrow button. Use the left arrow buttons to remove items from the Selected Prop-Sets list. For more information on creating Property Sets, see chapter 28.

   Optionally you can click the Table Specifications button to enter a heading, change the precision of the results, or specify the width of the tables generated in the report file.

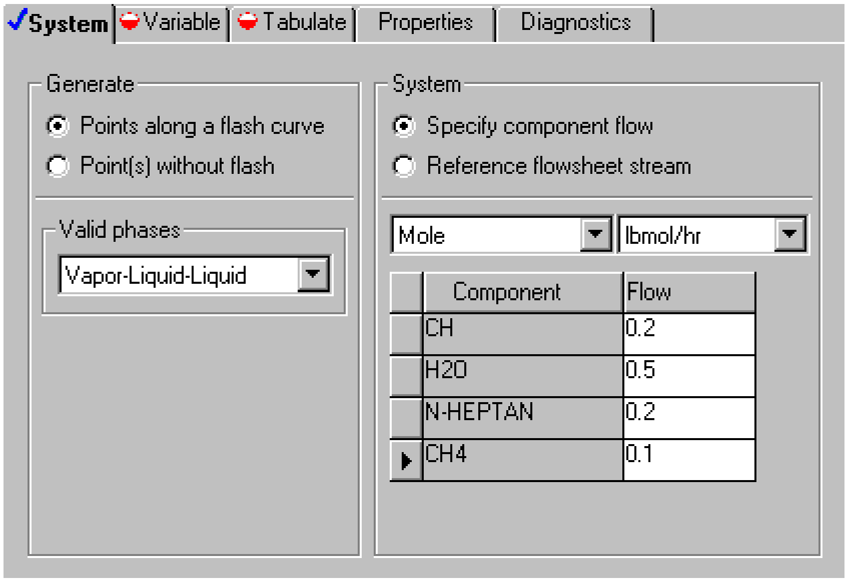
   Further optional specifications include:

   - Using the Properties sheet to change default property methods used to generate the generic Property Analysis.
   - Using the Diagnostics sheet to set how much information you receive about warnings and errors from calculations.

Results for the generic Analysis can be viewed on the Properties Analysis Generic Results form. For more information on Analysis results see Examining Property Analysis Results this chapter.

Example of Using Forms to Create a Generic Property Analysis to Study Rigorous 3-Phase Flash Behavior

Generate a table of properties at four pressures, using rigorous isothermal three-phase flash calculations. Tabulate vapor fraction, liquid-liquid ratio (beta), component mass fractions, and component flows for each of the three phases separately, and for the combined liquid phases.



Generate

● Points along a flash curve
○ Point(s) without flash

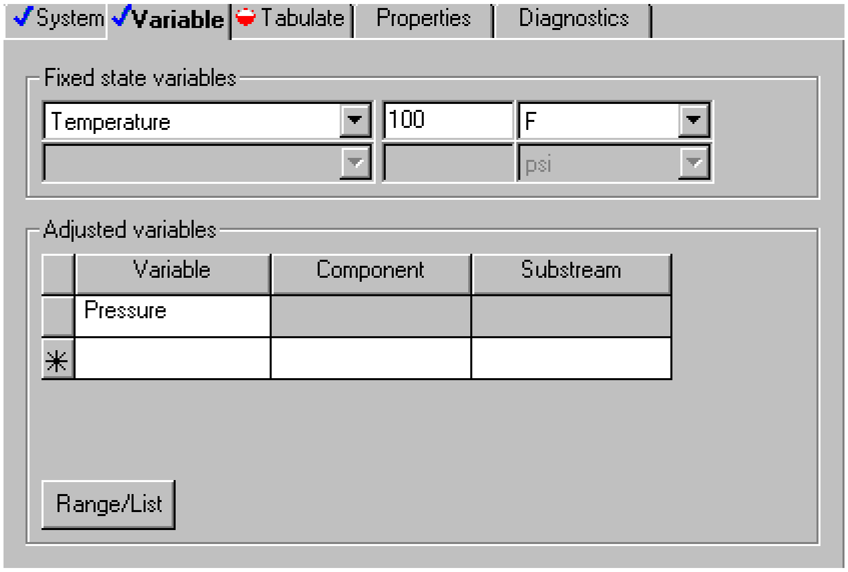
Valid phases: Vapor-Liquid-Liquid

System

● Specify component flow
○ Reference flowsheet stream

Mole
lbmol/hr

Component	Flow
CH	0.2
H2O	0.5
N-HEPTAN	0.2
CH4	0.1

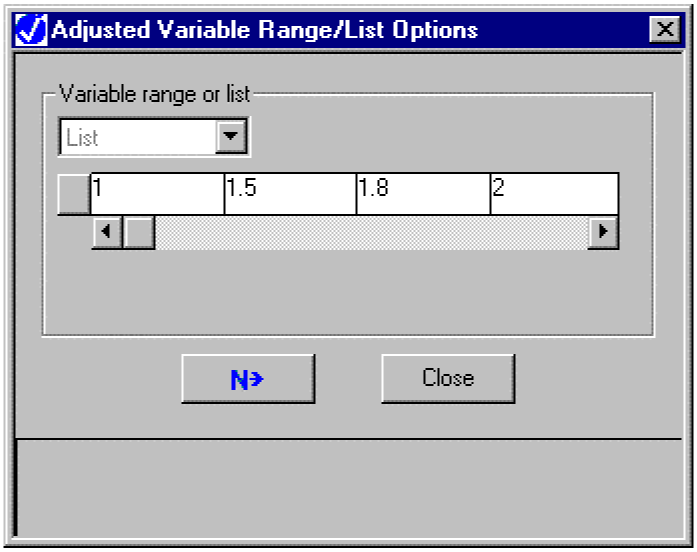


Fixed state variables

Temperature 100 F
psi

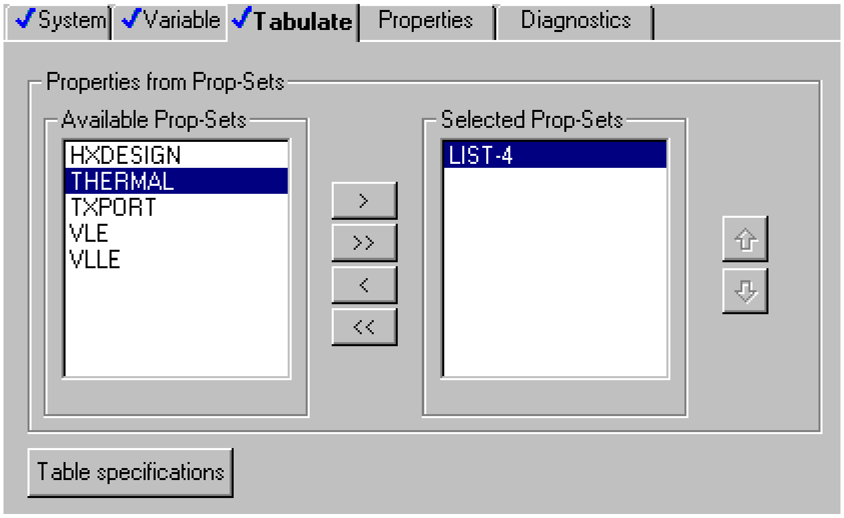
Adjusted variables

Variable	Component	Substream
Pressure		



Variable range or list: List

1	1.5	1.8	2

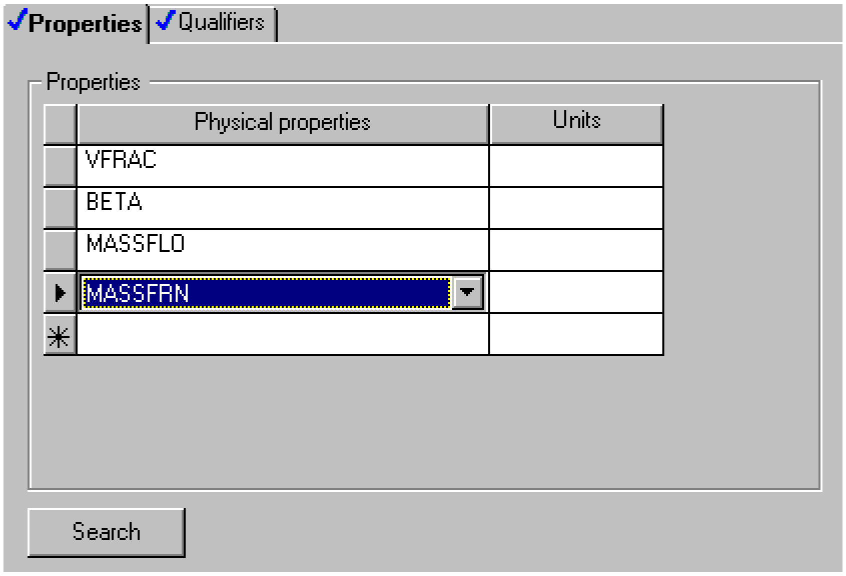


Properties from Prop-Sets

Available Prop-Sets:
- HXDESIGN
- THERMAL
- TXPORT
- VLE
- VLLE

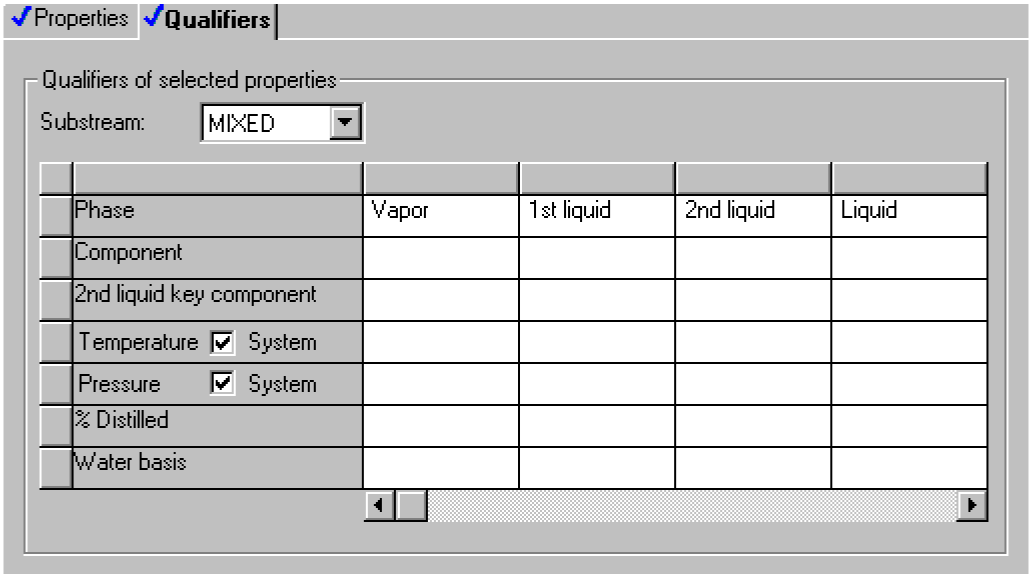
Selected Prop-Sets:
- LIST-4

The following two screens shows the property set, LIST-4, that defines the properties to be tabulated.



Properties

Physical properties	Units
VFRAC	
BETA	
MASSFLO	
MASSFRN	

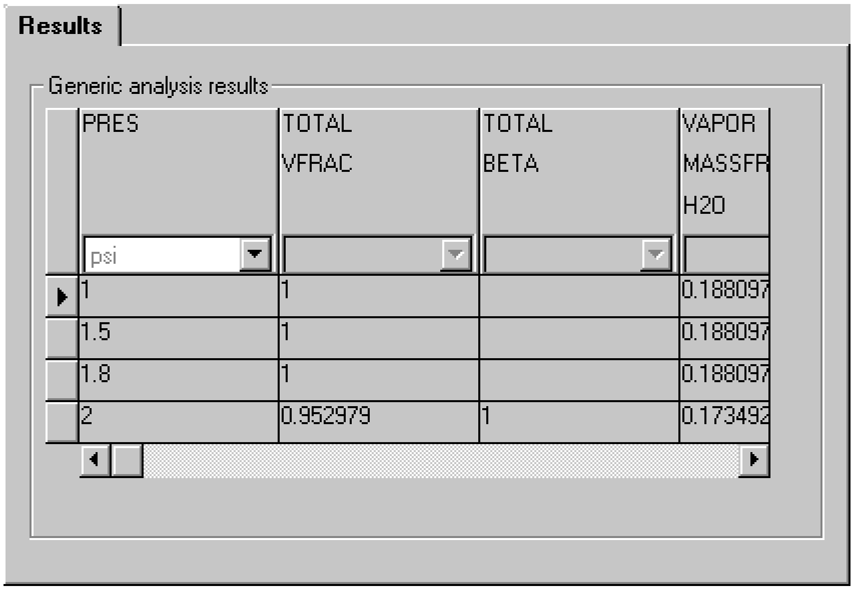


Qualifiers of selected properties

Substream: MIXED

Phase	Vapor	1st liquid	2nd liquid	Liquid
Component				
2nd liquid key component				
Temperature ☑ System				
Pressure ☑ System				
% Distilled				
Water basis				

Tabular results:



	PRES	TOTAL VFRAC	TOTAL BETA	VAPOR MASSFR H2O
	psi			
▶	1	1		0.188097
	1.5	1		0.188097
	1.8	1		0.188097
	2	0.952979	1	0.173492

To generate a plot of these results, select the variable on the Results sheet, then use Plot from the main menu bar to specify the x-axis or y-axis variable. Select Display Plot to view the plot.

Pressure-Temperature Envelopes

Use the PT-Envelope Property Analysis type to generate pressure-temperature envelopes. These tables are parametric, consisting of one curve for each vapor fraction, through the critical point, and its complementary vapor fraction. For example, the complementary branch for a vapor fraction of 0.75 is 0.25.

The interactive PT-Envelope Analysis command for streams also provides a complete facility for generating PT-Envelopes. Use the Property Analysis forms only if you want to tabulate properties in addition to temperature, pressure, and vapor fraction, or if you do not want to reference a stream.

You can generate PT-Envelopes from any property method except electrolyte property methods (for example, ELECNRTL). However, 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.

To generate a PT-Envelope using forms:

1. On the System sheet of the Properties Analysis PTEnvelope Input form, choose either to Specify Component Flow or Reference Flowsheet Stream. If you choose to specify component flow, enter the flow rates of your system. If you choose to reference a flowsheet stream, enter the Stream ID.
2. Click the Envelope sheet. By default this sheet is already complete.
3. On the Envelope sheet, specify the vapor fractions for which tables will be generated. By default, Aspen Plus generates the dew and bubble point curves (vapor fraction = 1 and 0, respectively.) You can specify additional vapor fractions. Aspen Plus generates one curve for each vapor fraction, through the critical point, and its complementary vapor fraction. For example, if you specify a vapor fraction of 0.25, Aspen Plus will generate one curve for the 0.25 and 0.75 vapor fraction branches.

   You can also specify these options:

   - Temperature or pressure of the first point
   - Maximum number of points
   - Termination point

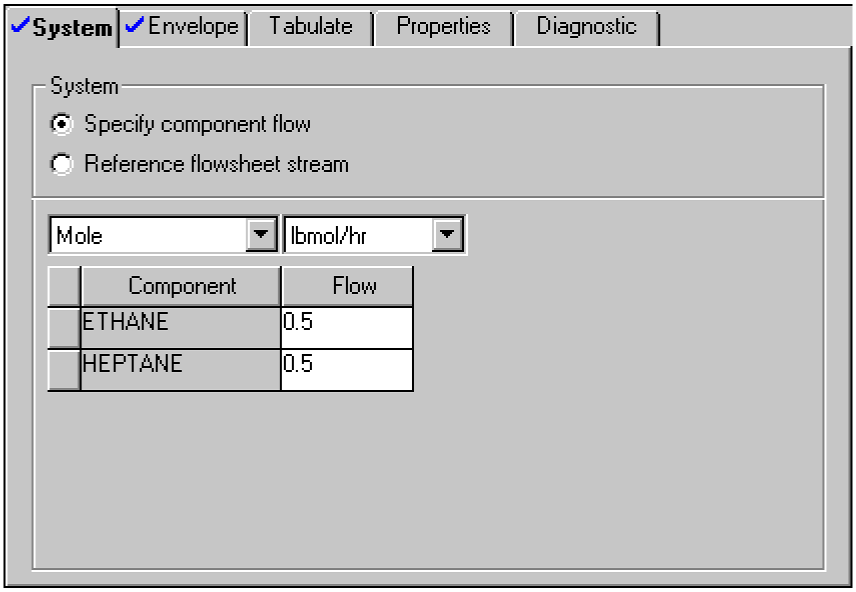
Further optional specifications include:

- Using the Tabulate sheet to specify properties to calculate in addition to the default temperature and pressure tabulations. Specify any additional properties by adding Property Set IDs to the Selected Prop-Sets list (see Chapter 28). You can also click the Table Specifications button to enter a heading, change the precision of the results, or specify the width of the tables generated in the Report file.
- Using the Properties sheet to change default property methods used to generate the PT envelope.
- Using the Diagnostics sheet to set how much information you receive about warnings and errors from calculations.

Results for the PT-Envelope can be viewed on the Properties Analysis PT-Envelope Results form. For more information on Analysis results see Examining Property Analysis Results this chapter.

Example of Using Forms to Generate a Pressure-Temperature Envelope

Generate a PT-Envelope for an equimolar mixture of ethane and n-heptane using the PENG-ROB property method. Generate the phase envelope for vapor fractions of 1, 0.5, and 0. Tabulate the mole fractions of the vapor and liquid phases, in addition to the default temperature and pressure.



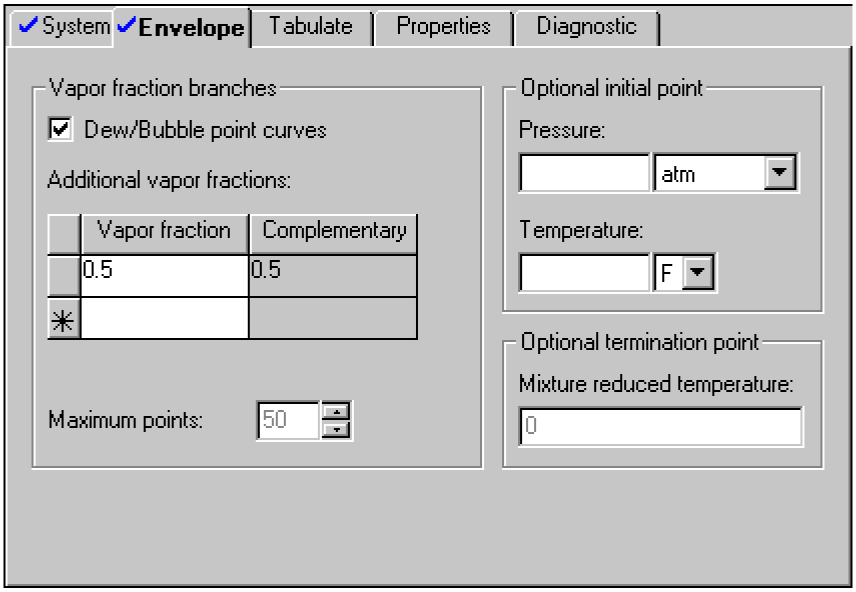
System

● Specify component flow

○ Reference flowsheet stream

Mole
lbmol/hr

Component	Flow
ETHANE	0.5
HEPTANE	0.5



Vapor fraction branches

☑ Dew/Bubble point curves

Additional vapor fractions:

Vapor fraction	Complementary
0.5	0.5

Maximum points: 50

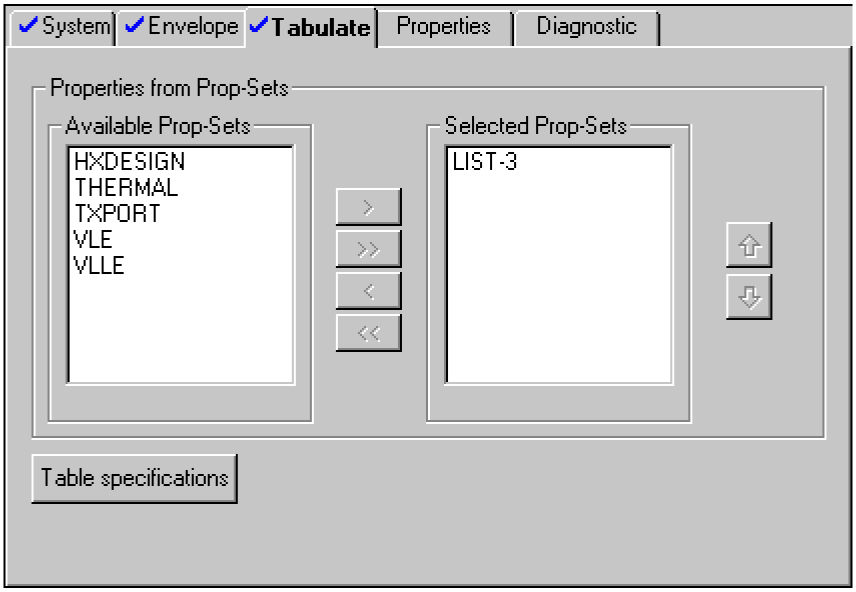
Optional initial point

Pressure: atm

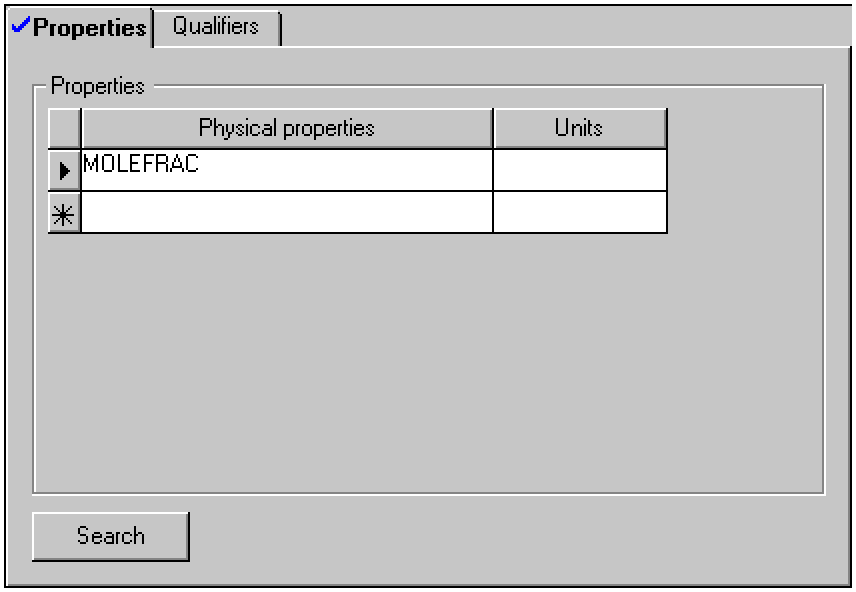
Temperature: F

Optional termination point

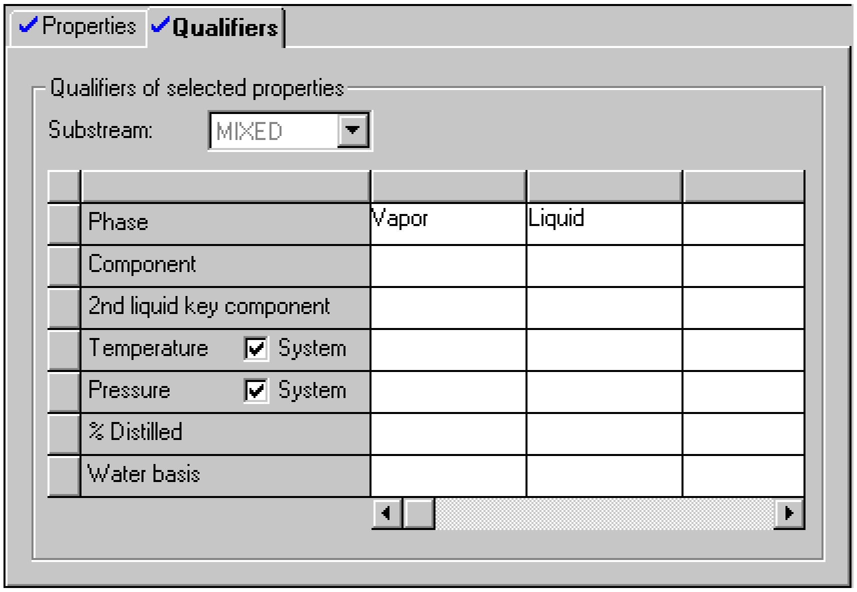
Mixture reduced temperature: 0



This is the property set, LIST-3, that defines the additional properties (mole fraction) to be tabulated:



	Physical properties	Units
▶	MOLEFRAC	
*		

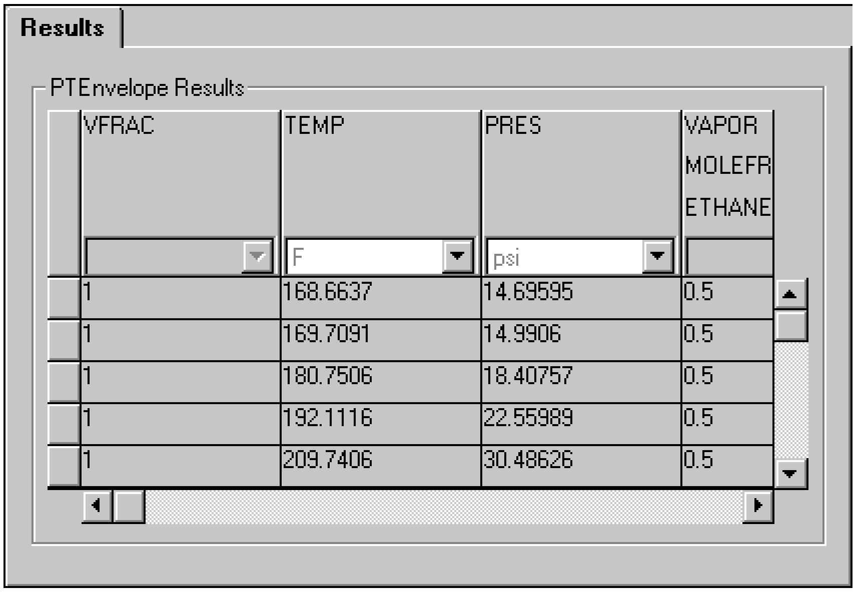


Qualifiers of selected properties

Substream: MIXED

Phase	Vapor	Liquid	
Component			
2nd liquid key component			
Temperature ☑ System			
Pressure ☑ System			
% Distilled			
Water basis			

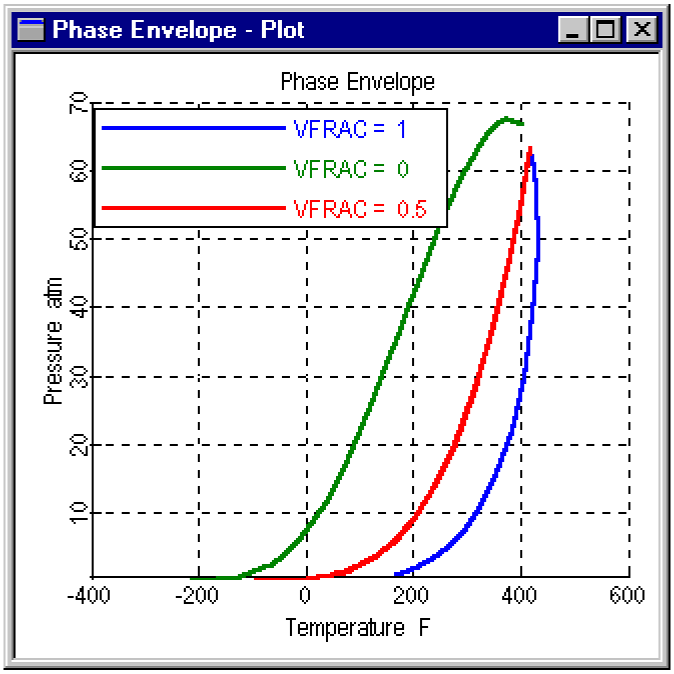
Tabular Results:



PTEnvelope Results

VFRAC	TEMP	PRES	VAPOR MOLEFR ETHANE
	F	psi	
1	168.6637	14.69595	0.5
1	169.7091	14.9906	0.5
1	180.7506	18.40757	0.5
1	192.1116	22.55989	0.5
1	209.7406	30.48626	0.5

To generate a plot of these results, choose Plot Wizard from the Plot menu of the main menu bar, while viewing the above results form. This is the resulting PT-Envelope plot, generated by accepting all the default settings of the Plot Wizard:



Residue Curves

Residue Curves (or maps) plot the composition trajectories of a ternary mixture undergoing distillation at total reflux. You can use them to visualize the presence of azeotropes and the constraints azeotropes impose on the degree of separation. Use Residue Curves to predict feasible splits, select entrainers, and analyze potential column operability problems (Doherty, 1978 and Wahnschaft, 1992).

Use Residue Curves with nonideal chemical systems, and Property Methods that represent such systems. Examples are activity-coefficient-based Property Methods, such as NRTL, Wilson, UNIQUAC, and UNIFAC.

To generate a Residue Curve using forms:

1. On the System sheet of the Properties Analysis Residue Input form, specify:
    - Components for the ternary mixture you want to analyze, using the Component 1, Component 2, and Component 3 list boxes.
    - System pressure using the Pressure field. The default is 1 atm.
    - Whether you want Aspen Plus to perform rigorous two-phase or three-phase calculations. Choose either Vapor-Liquid or Vapor-Liquid-Liquid in the Valid Phases list. The default is Vapor-Liquid.
    - Number of curves to be generated. Choose either 3-5 Curves, 10-15 Curves, or 15-20 Curves. Note that more curves require more calculation time. The default is 10-15 curves.

Optional specifications include:

- Using the Properties sheet to change default property methods used to generate the Residue Curve.
- Using the Diagnostics sheet to set how much information you receive about warnings and errors from calculations.

Results for the Residue Curve can be viewed on the Properties Analysis Residue Results form. For more information on Analysis results see Examining Property Analysis Results this chapter.

Property Methods Specifications for Property Analysis

Property Analyses use default property methods. Aspen Plus determines these defaults based on whether a flowsheet stream is referenced on the Property Analysis System form.

Flowsheet stream referenced?	Default property methods are
NO	Specified on the Properties Specifications Global sheet.
YES	The same as those used to calculate stream properties in the flowsheet simulation

You can override the default property specifications on the Properties Analysis Properties sheet.

Examining Property Analysis Results

To examine Property Analysis results:

1. From the Data menu, select Properties.
2. From the left pane of the Data Browser menu, double-click the Analysis folder.
3. Double-click the folder for the Property Analysis you wish to examine.
4. Click the Results folder.

You can plot the results using the Plot Wizard from the Plot menu of the main menu bar. For details on using the Plot Wizard, see chapter 13.

References

Doherty, M.F. and Perins, J.D., Chem. Eng. Sci., (1978), Vol. 33, p. 281.

Wahnschaft, O., "The Product Composition Regions of Single-feed Azeotropic Distillation Columns," Ind. Eng. Chem. Res., (1992), Vol. 31, pp. 2345-2362.

❖ ❖ ❖ ❖

30

Estimating Property Parameters

Aspen Plus stores physical property parameters in databanks for a large number of components. If a required parameter is not in any Aspen Plus databank, it can be:

- Entered directly (see Chapter 8)
- Estimated using Property Estimation
- Regressed from experimental data using Data Regression (see Chapter 31)

About Property Estimation

You can use Property Estimation in the following two ways:

- On a standalone basis
- In a Flowsheet, Property Analysis, PROPERTIES PLUS, or Data Regression run

This chapter includes the following information about estimating parameters using Property Estimation:

- Property parameters Aspen Plus can estimate
- Defining molecular structure
- Estimating parameters
- Using experimental data to improve estimated parameters
- Comparing estimated parameters for components
- Examining parameter estimation results

Property Estimation on a Standalone Basis

Property Estimation estimates all missing parameters listed in the tables on pages 30-3—30-6. To create a standalone estimation run, do one of the following:

- Select the Property Estimation Run Type when creating a new run.
- From the Data menu select Setup, then select the Specifications form. On the Global sheet, select Property Estimation in the Run Type list box.

Property Estimation in a Flowsheet, Property Analysis, PROPERTIES PLUS, or Data Regression Run

Property Estimation estimates all missing parameters from the tables on pages 30-3—30-6 that are required in the run.

When using Property Estimation in Flowsheet, Property Analysis, Data Regression, or Properties Plus run types, it is important understand which parameters will be used if a parameter is available from multiple sources.

If you select Estimate All Missing Parameters on the Estimation Input form, Aspen Plus will estimate and use all missing parameters that are required in the run. Parameters that are estimated, but are not missing, will not be used in the run.

If you selectively specify the estimation of an individual parameter that is required by the simulation, this estimated parameter will be used regardless of whether another value is available in a databank, or on a Properties Parameters input form.

What Property Parameters Can Aspen Plus Estimate?

Property Estimation in Aspen Plus can estimate many of the property parameters required by physical property models, including:

- Pure component thermodynamic and transport property model parameters
- Binary parameters for the Wilson, NRTL, and UNIQUAC activity coefficient models

The following tables list the property parameters Aspen Plus can estimate.

Property Names and Estimation Methods for Pure Component Constants

Description	Parameter	Method	Information Required†
Molecular weight	MW	FORMULA	Structure
Normal boiling point	TB	JOBACK OGATA-TSUCHIDA GANI MANI	Structure Structure Structure TC, PC, Vapor pressure data
Critical temperature	TC	JOBACK LYDERSEN FEDORS AMBROSE SIMPLE GANI MANI	Structure, TB Structure, TB Structure Structure, TB MW, TB Structure TC, PC, Vapor pressure data
Critical pressure	PC	JOBACK LYDERSEN AMBROSE GANI	Structure Structure, MW Structure, MW Structure
Critical volume	VC	JOBACK LYDERSEN AMBROSE RIEDEL FEDORS GANI	Structure Structure Structure TB, TC, PC Structure Structure
Critical compressibility factor	ZC	DEFINITION	TC, PC, VC
Standard heat of formation	DHFORM	BENSON JOBACK BENSONR8 GANI	Structure Structure Structure Structure
Standard Gibbs free energy of formation	DGFORM	JOBACK BENSON GANI	Structure Structure Structure
Acentric factor	OMEGA	DEFINITION LEE-KESLER	TC, PC, PL TB, TC, PC
Solubility parameter	DELTA	DEFINITION	TB, TC, PC, DHVL, VL
UNIQUAC R	UNIQUAC R	BONDI	Structure
UNIQUAC Q	UNIQUAC Q	BONDI	Structure
Parachor	PARC	PARACHOR	Structure
Solid enthalpy of formation at 25 C	DHSFRM	MOSTAFA	Structure
Solid Gibbs energy of formation at 25 C	DGSFRM	MOSTAFA	Structure

Continued

Property Names and Estimation Methods for Pure Component Constants (Continued)

Description	Parameter	Method	Information Required[†]
Aqueous infinite dilution Gibbs energy of formation for the Helgeson model	DGAQHG	AQU-DATA THERMO AQU-EST1 AQU-EST2	DGAQFM DGAQFM, S025C DGAQFM S025C
Aqueous infinite dilution enthalpy of formation for the Helgeson model	DHAQHG	AQU-DATA THERMO AQU-EST1 AQU-EST2	DGAQFM DGAQFM, S025C DGAQFM S025C
Entropy at 25 C for the Helgeson model	S25HG	AQU-DATA THERMO AQU-EST1 AQU-EST2	S025C DGAQFM, DHAQFM DGAQFM DHAQFM
Helgeson OMEGA heat capacity coefficient	OMEGHG	HELGESON	S25HG, CHARGE

[†] Structure *indicates that molecular structure must be defined using the Properties Molecular Structure forms. Data indicates that correlation parameters are determined directly from experimental data you enter on Properties Data forms. When another parameter is required, such as TB, it can come from a databank or from another estimation method. Or you can enter it on a Properties Parameters form.*

Property Names and Estimation Methods for Temperature-Dependent Properties

Description	Parameter	Method	Information Required[†]
Ideal gas heat capacity	CPIG	DATA BENSON JOBACK BENSONR8	Ideal gas heat capacity data Structure Structure Structure
Vapor pressure	PL	DATA RIEDEL LI-MA MANI	Vapor pressure data TB, TC, PC Structure, TB TC, PC, Vapor pressure data
Enthalpy of vaporization	DHVL	DATA DEFINITION VETERE GANI DUCROS LI-MA	Heat of vaporization data TC, PC, PL MW, TB Structure Structure Structure, TB
Liquid molar volume	VL	DATA GUNN-YAMADA LEBAS	Liquid molar volume data TC, PC, OMEGA Structure

Continued

Property Names and Estimation Methods for Temperature-Dependent Properties (Continued)

Description	Parameter	Method	Information Required[†]
Liquid viscosity	MUL	DATA ORRICK-ERBAR LETSOU-STIEL	Liquid viscosity data Structure, MW, VL, TC, PC MW, TC, PC, OMEGA
Vapor viscosity	MUV	DATA REICHENBERG	Vapor viscosity data Structure, MW, TC, PC
Liquid thermal conductivity	KL	DATA SATO-RIEDEL	Liquid thermal conductivity data MW, TB, TC
Vapor thermal conductivity	KV	DATA	Vapor thermal conductivity data
Surface tension	SIGMA	DATA BROCK-BIRD MCLEOD-SUGDEN	Surface tension data TB, TC, PC TB, TC, PC, VL, PARC
Solid heat capacity	CPS	DATA MOSTAFA	Solid heat capacity data Structure
Helgeson C heat capacity coefficient	CHGPAR	HG-AQU HG-CRIS HG-EST	OMEGHG, CPAQ0 OMEGHG, S25HG, CHARGE, IONTYP OMEGHG, S25HG
Liquid heat capacity	CPL	DATA RUZICKA	Liquid heat capacity data Structure

[†] Structure *indicates that molecular structure must be defined using the Properties Molecular Structure forms. Data indicates that correlation parameters are determined directly from experimental data you enter on Properties Data forms. When another parameter is required, such as TB, it can come from a databank or from another estimation method. Or you can enter it on a Properties Parameters form.*

In Flowsheet, Property Analysis, Properties PLUS, or Data Regression runs, Aspen Plus estimates missing binary parameters only if you request them on the Properties Estimation Input Binary sheet. If infinite dilution activity coefficients are estimated or supplied on the Properties Data Mixture form at only one temperature, then the parameters in brackets [ ] are set to zero.

Property Names and Estimation Methods for Binary Parameters

Description	Parameter	Method	Information Required[†]
Wilson parameters	WILSON/2 [WILSON/1]	DATA UNIFAC UNIF-LL UNIF- LBY UNIF- DMD UNIF-R4	Data Structure Structure Structure Structure Structure

Continued

Property Names and Estimation Methods for Binary Parameters (Continued)

Description	**Parameter**	**Method**	Information Required†
NRTL parameters	NRTL/2 [NRTL/1]	DATA UNIFAC UNIF-LL UNIF- LBY UNIF- DMD UNIF-R4	Data Structure Structure Structure Structure Structure
UNIQUAC parameters	UNIQ/2 [UNIQ/1]	DATA UNIFAC UNIF-LL UNIF- LBY UNIF- DMD UNIF-R4	Data Structure, GMUQR, GMUQQ Structure, GMUQR, GMUQQ Structure, GMUQR, GMUQQ Structure, GMUQR, GMUQQ Structure, GMUQR, GMUQQ

† Structure *indicates that molecular structure must be defined using the Properties Molecular Structure forms. Data indicates that correlation parameters are determined directly from experimental data you enter on Properties Data forms. When another parameter is required, such as TB, it can come from a databank or from another estimation method. Or you can enter it on a Properties Parameters form.*

Property Names and Estimation Methods for UNIFAC Group Parameters

Description	Parameter	Method	Information Required†
UNIFAC R	UNIFACR	BONDI	Structure
UNIFAC Q	UNIFACQ	BONDI	Structure
Lyngby UNIFAC R	UNIFLR	BONDI	Structure
Lyngby UNIFAC Q	UNIFLQ	BONDI	Structure
Dortmund UNIFAC R	UNIFDR	BONDI	Structure
Dortmund UNIFAC Q	UNIFDQ	BONDI	Structure

† Structure *indicates that molecular structure must be defined using the Properties Molecular Structure forms. Data indicates that correlation parameters are determined directly from experimental data you enter on Properties Data forms. When another parameter is required, such as TB, it can come from a databank or from another estimation method. Or you can enter it on a Properties Parameters form.*

Required Information for Parameter Estimation

The minimum information required for parameter estimation is:

- Normal boiling point temperature (TB)
- Molecular weight (MW)
- Molecular structure, preferably entered using the General method

Property Estimation uses normal boiling point and molecular weight to estimate many parameters. You can greatly reduce the propagation of errors in estimating other parameters by using the experimental value of TB. If you do not supply TB and MW but you enter the general molecular structure, Property Estimation can estimate TB and MW.

To obtain the best possible estimates for all parameters, enter all the experimental data that is available.

Defining Molecular Structure Using the General Method

When you use the general method to describe the atoms and bonds in a compound, Aspen Plus automatically generates the required functional groups for the estimation methods used in a particular run.

To use the general method:

1. Sketch the structure of the molecule on paper.
2. Assign a number to each atom, omitting hydrogen. The numbers must be consecutive, starting from 1.
3. From the Data menu, click Properties.
4. In the left pane of the Data Browser, click Molecular Structure.
5. From the Molecular Structure Object Manager, select a component ID for which you want to specify the molecular structure, then click Edit.

On the General sheet, define the molecule by its connectivity, one pair of atoms at a time.

In this field	Enter
Number	Unique number identifying an atom in the molecule. This should be the atom number that you assigned in your preliminary drawing.
Type	Atom type (for example, carbon or oxygen)
Bond type	Type of bond that connects a pair of atoms (for example, single or double)

Atom numbers and atom types appear on the correspondence list at the bottom of the form.

Atoms Numbers and Types

When you enter an existing atom number, Aspen Plus displays the atom type (except for the first pair of atoms). You can omit specifying values in the Number and Type fields for the first atom of a pair. Aspen Plus will automatically use the atom number and type of the second atom for the previously entered pair. Enter a number for the second atom of the current pair.

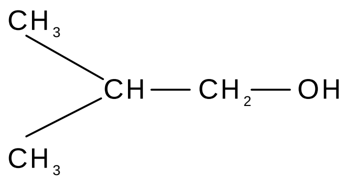
You can use the following bond types to simplify the task of entering the structure of common ring compounds and saturated hydrocarbons:

Special Bond Type	Description
Benzene ring	Benzene ring
Sat. 5-member ring	Saturated 5-member ring
Sat. 6-member ring	Saturated 6-member ring
Sat. 7-member ring	Saturated 7-member ring
Sat. hydrocarbon chain	Saturated hydrocarbon chain

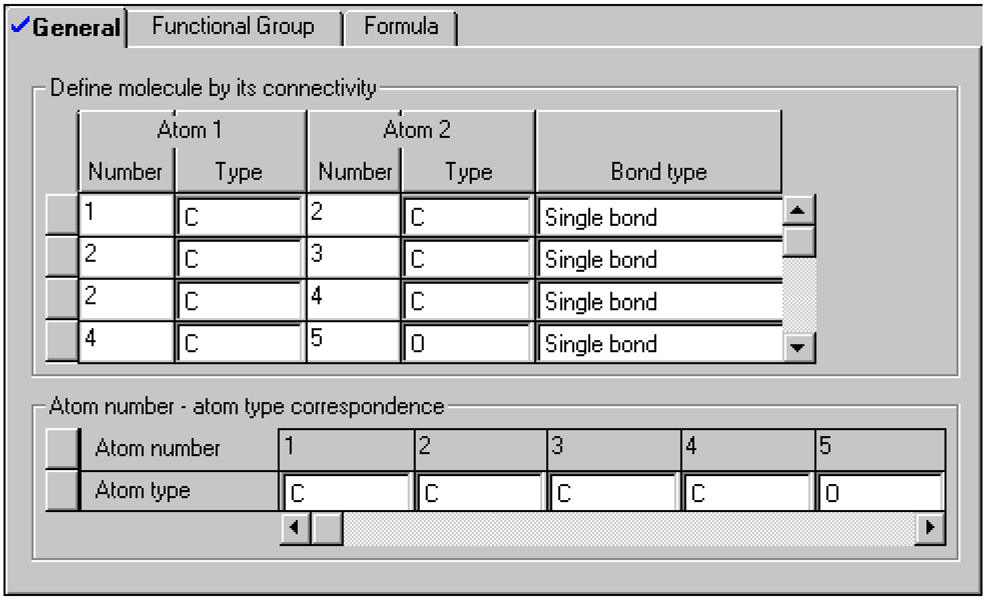
When you use these special bond types, the atom numbers assigned to the members of the carbon ring or carbon chain must be consecutive.

Example of Defining Molecular Structure Using the General Method

Define the molecular structure of isobutyl alcohol (C4H10O) using the general method.



Assign a number to each atom, omitting hydrogen.



Define molecule by its connectivity

Atom 1		Atom 2		
Number	Type	Number	Type	Bond type
1	C	2	C	Single bond
2	C	3	C	Single bond
2	C	4	C	Single bond
4	C	5	O	Single bond

Atom number - atom type correspondence

Atom number	1	2	3	4	5
Atom type	C	C	C	C	O

Defining Molecular Structure Using Method-Specific Functional Groups

Use the Properties Molecular Structure Functional Group sheet to enter method-specific functional groups. For each group-contribution method, specify:

- Functional groups
- Number of times each group occurs in the compound

Functional groups are defined and numbered differently for each method. For functional group definitions, see *Aspen Plus Physical Property Data*, or browse through the Group Number list.

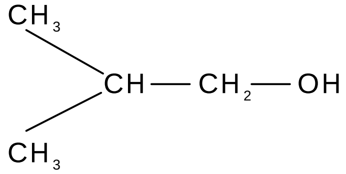
You can enter any number of pairs for group numbers and number of occurrences, with one exception. For the UNIFAC, UNIF-LL, UNIF-DMD, and UNIF-LBY methods the limit is 12.

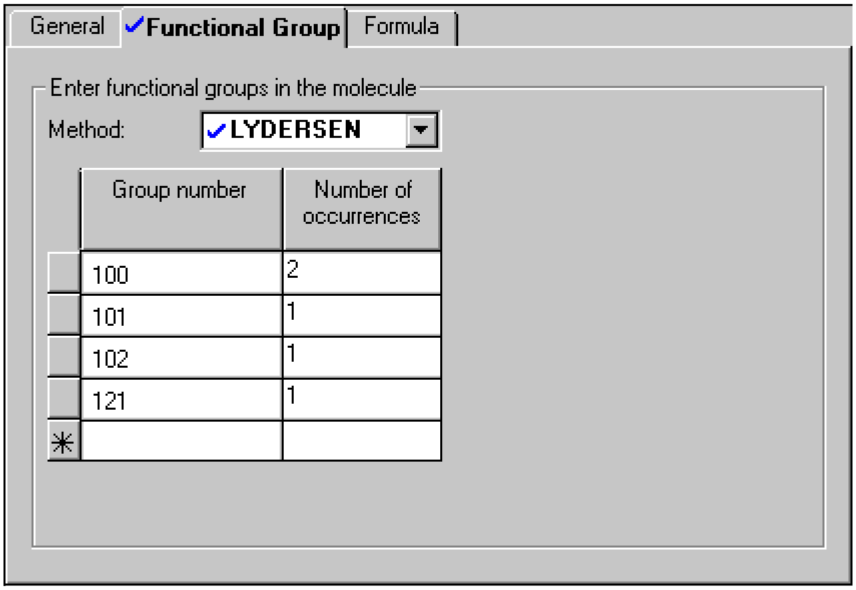
To specify method specific functional groups:

1. Sketch the structure of the molecule on paper.
2. From the Data menu, click Properties.
3. In the left pane of the Data Browser, click Molecular Structure.
4. From the Molecular Structure Object Manager, select a component ID for which you want to specify the molecular structure, then click Edit.
5. Click the Functional Group sheet.
6. On the Functional Group sheet, select the estimation method from the Method list box.
7. In the Group Number list, select a functional group for the method, that represents a functional group contained in your molecule. The prompt area displays a description of the functional group.
8. Count the number of times this group occurs in the molecule and enter that number in the Number of Occurrences field. The default is one.
9. Repeat steps 7 and 8 until all functional groups in your molecule are represented with the appropriate number of occurrences.

Example of Defining Molecular Structure Using Method-Specific Functional Groups

The structure of isobutyl alcohol is defined using the Lydersen method. The Lydersen functional groups are -CH3, >CH2, >CH-, and -OH. The corresponding group numbers are 100, 101, 102, and 121, respectively.





Enter functional groups in the molecule

Method: ✓LYDERSEN

Group number	Number of occurrences
100	2
101	1
102	1
121	1

Identifying Parameters to be Estimated

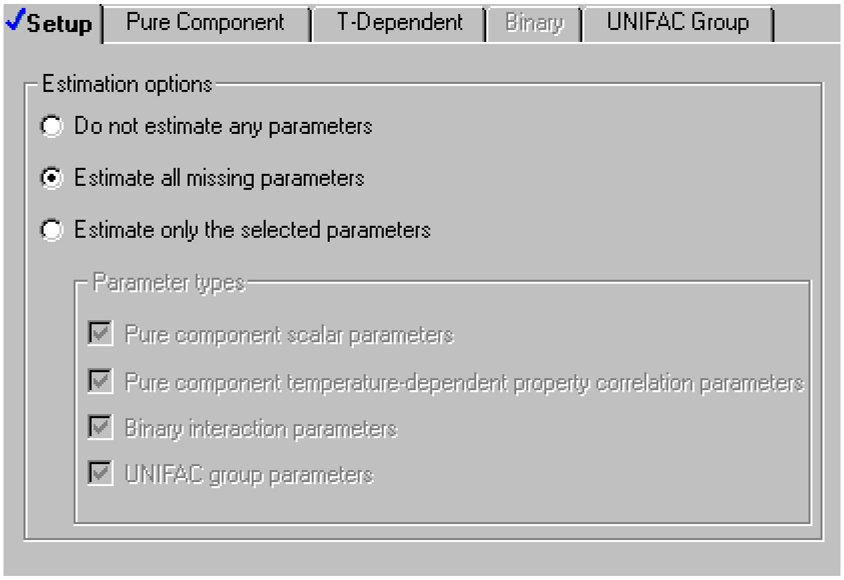
In a standalone Property Estimation run, Aspen Plus estimates all missing parameters listed in the tables on pages 30-3—30-6, using default methods. You can use the Properties Estimation Input form to request parameter estimation and to:

- Specify the properties and components for which parameters are to be estimated
- Select estimation methods
- Request estimation for parameters that are not missing

In a Flowsheet, Data Regression, or Property Analysis run, you must request estimation of missing parameters. Aspen Plus estimates all missing required parameters using default methods, unless you specify otherwise on the Input form.

To request parameter estimation:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser Menu, select Estimation then Input.



Estimation options

○ Do not estimate any parameters

● Estimate all missing parameters

○ Estimate only the selected parameters

Parameter types

☑ Pure component scalar parameters

☑ Pure component temperature-dependent property correlation parameters

☑ Binary interaction parameters

☑ UNIFAC group parameters

3. On the Setup sheet, specify one of the following Estimation options.

Option	Estimates
Do not estimate any parameters	Nothing. This is the default.
Estimate all missing parameters	All missing required parameters and any parameters you request on the Pure Component, T-Dependent, Binary, and UNIFAC Group sheets
Estimate only the selected parameters	Only the types of parameters you specify on the Setup sheet. Specific estimations must be specified on the sheets identified by your parameter types selection on this sheet.

The Estimate All Missing Parameters option is strongly recommended unless you:

- Know exactly what parameters are missing and want to estimate only those parameters
- Want to evaluate the estimation methods only for certain parameters

4. If you selected Estimate Only the Selected Parameters, specify the type(s) of parameters to estimate by checking the appropriate checkboxes. Go to the appropriate sheet to specify the desired parameters and methods.

   You must supply all information required to estimate the parameters.

5. If you selected Estimate All Missing Parameters, you can override default estimation methods. Go to the appropriate sheet to specify parameters and methods for the different types of parameters.

Use these sheets to select parameters and methods:

Form	What is Specified
Pure Component	Parameter names and estimation methods for pure component constants
T-Dependent	Parameter names and estimation methods for temperature-dependent parameters
Binary	Parameter names and estimation methods for binary parameters
UNIFAC Group	Parameter names for UNIFAC group parameters

See subsequent sections of this chapter for more information on these sheets.

When using Property Estimation in Flowsheet, Property Analysis, Data Regression, or Properties Plus run types, if you manually request the estimation of specific parameters using the sheets in the table above, these estimated values are used preferentially over any values available in a databank or on a Properties Parameters form.

You can specify more than one estimation method for a parameter. This allows you to compare the estimates predicted by different methods.

When you specify multiple estimation methods for a parameter required in a Flowsheet, Property Analysis, Data Regression, or Properties Plus run type, the simulation uses the value estimated by the first estimation method selected.

The tables on pages 30-3—30-6 list the estimation methods Aspen Plus provides for each parameter. For details on the accuracy and applicability of each estimation method, see *Aspen Plus Physical Property Methods and Models,* Chapter 8.

Estimating Pure Component Parameters

Use the Estimation Input Pure Component sheet to request estimation of pure component constants, such as critical temperature (TC).

To request estimation of a pure component constant:

1. From the Data menu, click Properties
2. In the left pane of the Data Browser Menu, select Estimation, then Input.
3. On the Setup sheet, choose estimation options. For more information, see Identifying Parameters to be Estimated on page 30-11.
4. Click the Pure Component sheet.
5. On the Pure Component sheet, select a parameter you want to estimate using the Parameter list box.

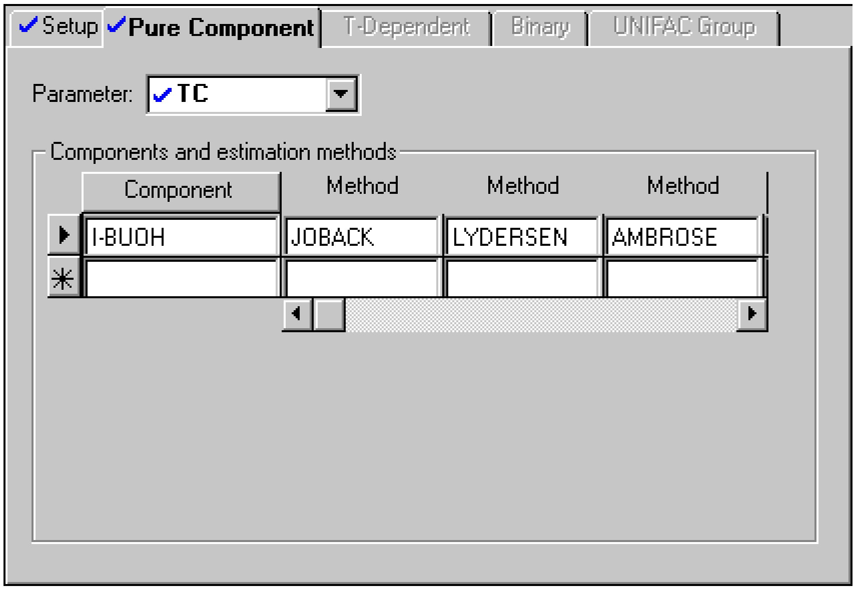
6. In the Component list box, select the component for which you want to estimate the selected parameter. If you want to estimate the chosen parameter for multiple components, you may continue to select additional components individually, or you may select All to estimate the parameter for all components.
7. In the Method list box for each selected component, choose the estimation method you want to use. You can specify more than one method.
8. To request estimation of additional pure component parameters, select a different parameter in the Parameter list box, and repeat steps 6 and 7.

If you specify more than one method, only the value estimated by the first method is used. Results for all the methods specified are displayed on the Estimation Results form. See Examining Parameter Estimation Results on page 30-22.

The only reason for specifying more than one method is to evaluate the accuracy of methods used in estimating a given parameter. See Comparing Estimated Parameters to Experimental Data on page 30-21.

Example for Estimating Critical Temperature

This estimation problem is set up to evaluate the accuracy of three methods (Joback, Lydersen, and Ambrose) for estimating TC for isobutyl alcohol:



Parameter: ✓TC

Component	Method	Method	Method
I-BUOH	JOBACK	LYDERSEN	AMBROSE

Estimating Temperature-Dependent Properties

Use the Estimation Input T-Dependent sheet to request estimation of correlation parameters for temperature-dependent properties (such as parameters for the extended-Antoine vapor pressure). Property Estimation uses estimation methods based on group contributions and corresponding-states theory. In addition, Property Estimation accepts experimental property versus temperature data and uses them to determine the correlation parameters by regression.

To request estimates of temperature-dependent properties:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser, click the Estimation subfolder.
3. On the Setup sheet, choose estimation options. For more information, see Identifying Parameters to be Estimated on page 30-11.
4. Click the T-Dependent sheet.
5. On the T-Dependent sheet, specify the property you want to estimate in the Property list box.
6. In the Component list box, select the component for which you want to estimate the selected property. If you want to estimate the chosen property for multiple components, you may continue to select additional components individually, or you may select All to estimate the property for all components.
7. In the Method list box for each selected component, choose the estimation method you want to use. You can specify more than one method for each property. To do this, list the component again, and choose a different method.
8. To request estimation of additional temperature dependent properties, select a different property in the Property list box, and repeat steps 6 and 7.

   If you specify more than one method for a component, only the estimated value of the first method is used. Results for all the methods specified are displayed on the Results form. See Examining Parameter Estimation Results on page 30-22.

   The only reason for specifying more than one method is to evaluate the accuracy of methods used in estimating a given property. See Comparing Estimated Parameters to Experimental Data on page 30-21.
9. If you want to restrict estimation to a temperature range, enter the lower temperature limit in the Lower Temp. field, and enter the upper temperature limit in the Upper Temp. field.
10. If you have experimental property versus temperature data, enter them on the Properties Data Pure-Comp form.

When you select	Then Aspen Plus
DATA in the Method field	Uses the experimental data you enter on the Properties Data Pure-Comp form to determine the correlation parameters by regression
DATA in the Method field, and Upper Temp. and Lower Temp.	Uses only the experimental data within the temperature ranges you specify
A method other than DATA	Uses the specified method to estimate the property over a range of temperatures (Upper Temp. and Lower Temp.). Aspen Plus determines the correlation parameters that best fit the estimated data
A method other than DATA and you check the Use Data check box	Combines the experimental data you enter on the Properties Data Pure-Comp form with the estimated values using the method you specified to determine the best correlation parameters

If you combine the experimental data and estimated values (by selecting the Use Data check box), you can assign a weight to the experimental data in the Weight field. The weight is relative to 1.0 for estimated values.

Estimating Binary Parameters

Use the Estimation Binary Input sheet to request estimates of binary parameters, such as WILSON/1 and WILSON/2 for the Wilson model. Aspen Plus estimates binary parameters using infinite-dilution activity coefficient data.

To request estimates of binary parameters:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser Menu, click Estimation then Input.
3. On the Setup sheet, choose estimation options. For more information, see Identifying Parameters to be Estimated on page 30-11.
4. Click the Binary sheet.
5. On the Binary sheet, click New then specify the parameter you want to estimate in the Parameter list box.
6. In the Method list box, choose the estimation method you want to use. You can specify more than one method for each parameter.

When Method is	Then Aspen Plus uses
DATA	The infinite dilution activity coefficient data you enter on the Properties Data Mixture form. For more information see Using Infinite Dilution Activity Coefficient Data on page 30-20.
A method other than DATA	The method to estimate infinite dilution activity coefficients

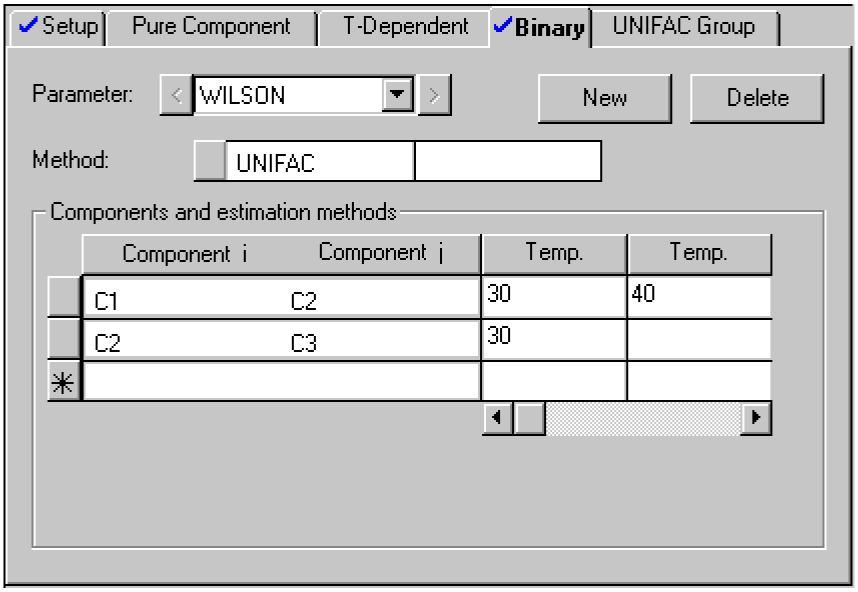
7. In the Component i and Component j list boxes, specify two components for which you want to estimate interaction parameters. If you want to estimate the chosen parameter for multiple component pairs, you may continue to select additional component pairs individually, or you may select All to estimate the parameters for all component pairs.
8. In the Temp field, you can specify the temperature(s) of the infinite-dilution activity coefficient data. The default temperature is 25 C. If you select DATA in the Method field, the default is all the data you entered on the Properties Data Mixture form.

When you	Aspen Plus estimates
Enter no temperature value, or enter only one temperature value	Only the second element of the parameter (for example, WILSON/2 for Wilson)
Enter more than one temperature value	Elements one and two of the parameter (for example, WILSON/1, WILSON/2)

9. To request estimation of additional binary parameters, select a different parameter in the Parameter list box, and repeat steps 6, 7 and 8.

Example for Estimating Binary Parameters

Estimate Wilson binary parameters from infinite-dilution activity coefficients generated by UNIFAC. Estimate the infinite-dilution activity coefficients at 30 and 40°C for component pair C1-C2; and at 30°C for component pair C2-C3. For C1-C2, the WILSON/1 and WILSON/2 binary parameters are estimated because two temperatures are requested. For C2-C3, only the WILSON/2 parameter is estimated because only one temperature is requested.



Parameter: WILSON

Method: UNIFAC

Component i	Component j	Temp.	Temp.
C1	C2	30	40
C2	C3	30	

Estimating UNIFAC Group Parameters

Use the Properties Estimation UNIFAC Group sheet to request parameter estimation for UNIFAC functional groups. Group parameters for all UNIFAC groups are built into Aspen Plus. You do not need to estimate them.

If you define a new UNIFAC group on the Components UNIFAC-Groups form:

Use this sheet	To
Properties Molecular Structure Functional Group	Define the structure of the UNIFAC group using the Bondi method
Properties Estimation Input UNIFAC Group	Estimate group parameters

To request parameter estimation for UNIFAC functional groups:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser Menu, select Estimation then Input.
3. On the Setup sheet, choose estimation options. For more information, see Identifying Parameters to be Estimated on page 30-11.
4. Click the UNIFAC Group sheet.
5. In the Parameter list box, specify the UNIFAC group parameter you want to estimate .
6. In the Group ID fields, enter the UNIFAC Group IDs for which you want to estimate parameters.

   UNIFAC group IDs must have been defined on the Components UNIFAC-Groups form.

Using Experimental Data to Improve Estimated Parameters

You can use any experimental property data available to improve the quality of your parameter estimation. Whenever possible, supply experimental data to minimize the propagation of errors due to the uncertainty of estimated values.

Temperature-dependent property data (such as vapor pressure versus temperature data) can be used directly to determine correlation parameters by regression. Infinite-dilution activity coefficient data are used to estimate binary parameters.

Use this form	To enter this type of property data
Properties Parameters Pure Component Scalar	Scalar property constants, such as normal boiling point (TB) or critical temperature (TC) (See Chapter 8)
Properties Parameters Pure Component T-Dependent	Temperature-dependent correlation parameters, such as PLXANT for the extended Antoine vapor pressure model (See Chapter 8)
Properties Data PURE-COMP	Temperature-dependent property data, such as vapor pressure versus temperature points (See Chapter 31))
Properties Data MIXTURE	Infinite dilution activity coefficient data versus temperature for binary systems (See Chapter 31)

Using Temperature-Dependent Property Data

Use the Properties Data PURE-COMP form to enter temperature-dependent property data.

Enter the data as pairs of temperature and property values.

To enter temperature-dependent property data: listed in the table on page 30-4:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser, click the Data subfolder.
3. To create a new Data ID, on the Data Object Manager, click New.
4. In the Create New ID dialog box, enter an ID for the data, or accept the default ID. Choose PURE-COMP from the Select Type list box, and click OK.
5. To modify an existing Data ID, select the ID from the Data Object Manager, and click Edit.
6. On the Setup sheet, select the category For Estimation, then specify the property for which you have data, in the Property list box.
7. Select the component for which you have data, in the Component list box.
8. If your data was measured at a constant temperature or pressure, you can enter this value in the Constant Temperature or Pressure frame.
9. Click the Data sheet.
10. On the Data sheet, enter the experimental data in the appropriate columns. The first column in the data table, Usage, will be filled in automatically when you begin entering your data points.

    The first row of the data table is filled in with default values of standard deviation. These standard deviations are not considered in Property Estimation however. They are only used in Data Regression. (See Chapter 31)

To combine the experimental pure component data to estimate temperature-dependent property parameters:

1. Select the Properties Estimation Input T-Dependent sheet.
2. Select the property you wish to estimate in the Property list box.
3. Specify the component then select DATA in the Method list box.

You can combine experimental temperature-dependent property data with estimated data. For example, you can combine experimental vapor pressure data with values estimated by the Riedel method. The combined data are then used to determine the best set of PLXANT parameters. You can use this feature to extrapolate limited experimental data. For more information, see Estimating Temperature-Dependent Properties on page 30-15.

The experimental data you enter can be used in three ways:

- By Data Regression, to obtain correlation parameters by regression.
- By Property Estimation, to obtain correlation parameters by regression.
- By Property Estimation, together with other estimated values, to obtain correlation parameters.

Using Property Estimation is similar to using Data Regression to regress pure component temperature-dependent property data or infinite-dilution activity coefficient data. However, with Data Regression you can:

- Mix VLE and pure component data
- Regress any parameter, such as an equation-of-state parameter
- Control which parameters in a correlation to regress
- Provide standard deviations (weightings) for individual variables and data points

For detailed information about data regression, see Chapter 31.

Using Infinite Dilution Activity Coefficient Data

Use the Properties Data MIXTURE form to enter infinite-dilution activity coefficient (gamma infinity) data for binary systems.

To enter infinite-dilution activity coefficient data:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser Menu, select the Data subfolder.
3. To create a new Data ID, on the Data Object Manager, click New. On the Create New ID dialog box, enter an ID for the data, or accept the default ID. Choose MIXTURE from the Select Type list box, and click OK.
4. To modify an existing Data ID, select the ID from the Data Object Manager, and click Edit.

5. On the Setup sheet, select the category For Estimation in the category list box, then GAMINF in the Data Type list box.
6. Select the components for which you have data from the Available Components list, and use the right arrow button to move the two components of interest to the Selected Components list.
7. Click the Data sheet.
8. On the Data sheet, enter the experimental data in the appropriate fields as described in the table below. The first column in the data table, Usage, will be filled in automatically when you begin entering your data points.

   The first row of the data table is filled in with default values of standard deviation. These standard deviations are not considered in Property Estimation however. They are only used in Data Regression. (See Chapter 31)

Field	Enter
TEMP1	Temperature corresponding to the infinite-dilution activity coefficient of component 1 (GAMINF1)
GAMINF1	Infinite-dilution activity coefficient of component 1
TEMP2	Temperature corresponding to the infinite-dilution activity coefficient of component 2 (GAMINF2)
GAMINF2	Infinite-dilution activity coefficient of component 2

   If one infinite-dilution activity coefficient value is missing, leave both the TEMP and GAMINF fields blank.

To use the experimental infinite-dilution activity coefficient data to estimate binary parameters:

1. Select the Properties Estimation Input Binary sheet.
2. Select the parameter you want to estimate in the Parameter list box.
3. Select DATA in the Methods list box.
4. In the Component i and Component j fields, specify the two components for which you have entered infinite-dilution activity coefficient data.

Comparing Estimated Parameters to Experimental Data

Use the Properties Estimation Compare form to compare estimated parameters to experimental data. You can also compare the estimated values of components to results for other components. This feature can help you select the best method for estimating parameters for a nondatabank component when only limited experimental data is available.

To evaluate the accuracy of estimation methods used for a parameter and to select the best methods for estimating parameters for a nondatabank component:

1. Identify databank components that are similar to the nondatabank component in terms of molecular structure or functional groups.
2. Request parameter estimation for these databank components using all methods available on the Estimation Input form.
3. Use the Estimation Compare form to compare the estimated parameters to the experimental data.

From the comparison you can determine the best method for each parameter. The best methods for the databank components should also be best for the nondatabank component.

To compare estimated parameters to experimental data:

1. From the Data menu, click Properties
2. In the left pane of the Data Browser Menu, double-click the Estimation subfolder.
3. Select the Compare form.
4. On the Compare Setup sheet, use the Components and UNIFAC Group IDs list boxes to enter components or groups to be compared with experimental data.

Examining Parameter Estimation Results

To examine parameter estimation results:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser Menu, double-click the Estimation subfolder.
3. Select the Results or the Compare Results form.

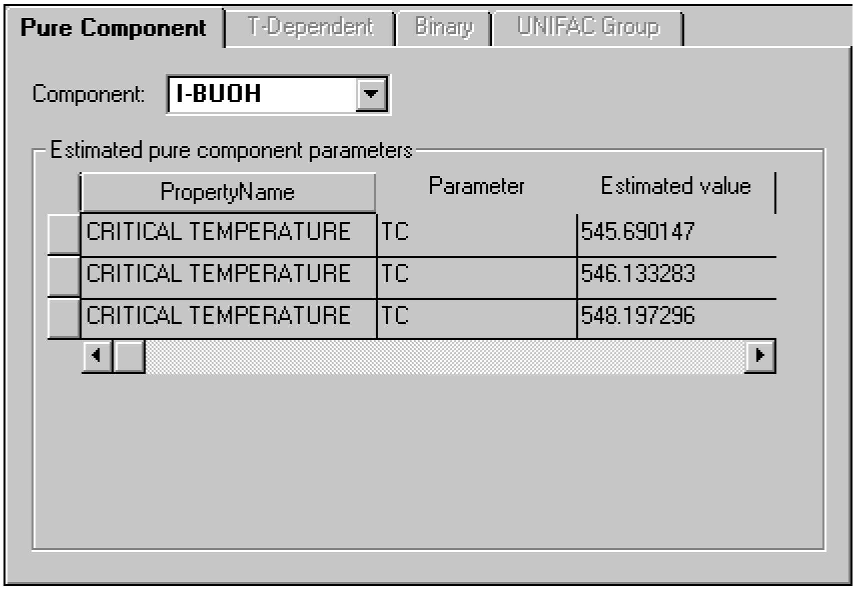
The Estimation Results form displays the estimated properties and parameters that you requested on the Estimation Input form. Estimated parameters are also placed on appropriate Properties Parameters forms. The Compare Results form displays comparisons between estimated and experimental data , as requested on the Estimation Compare form. Comparisons between components are not displayed on the Compare Results form, they are contained in the reports.

To view comparisons between components:

From the View menu, click Reports.

Example of Pure Component Estimation Results

This example shows the estimated values of TC for isobutyl alcohol using three methods (Joback, Lydersen, and Ambrose).



Component: I-BUOH

Estimated pure component parameters

PropertyName	Parameter	Estimated value
CRITICAL TEMPERATURE	TC	545.690147
CRITICAL TEMPERATURE	TC	546.133283
CRITICAL TEMPERATURE	TC	548.197296

Using Estimated Parameters

If you estimate parameters, you can choose whether the results are automatically written to Properties Parameters input forms or not.

If you estimate parameters in a standalone Property Estimation run, and then want to use them in a Flowsheet, Property Analysis, Data Regression, or Properties Plus run:

- ➤ On the Setup Specifications Global sheet, change the Run Type.

When using Property Estimation in Flowsheet, Property Analysis, Data Regression, or Properties Plus runs, if you select Estimate All Missing Parameters, Aspen Plus estimates and uses all missing parameters that are required in the run. Aspen Plus does not estimate any parameters that are not missing.

If you specifically request the estimation of an individual parameter, this estimated parameter will be used preferentially over any databank value, or any value entered on Properties Parameters forms.

Saving Estimation Results Automatically

If you estimate parameters, by default the results are automatically written to Properties Parameters input forms.

This means that when you are satisfied with your estimation results, you can turn off Property Estimation because the estimated parameters have been preserved on the Parameters forms for use in subsequent simulation runs.

To turn off Property Estimation:

➤ On the Setup sheet of the Properties Estimation Input form, check Do Not Estimate Any Parameters.

Not Saving Estimation Results Automatically

If you do not want the estimation results to be written to the Parameters forms automatically:

1. From the Tools menu, click Options.
2. Click the Component Data tab.
3. Clear the Copy Regression and Estimation Results onto Parameters Forms checkbox.

❖ ❖ ❖ ❖

31 Regressing Property Data

You can use experimental property data to determine the physical property model parameters you need for an Aspen Plus simulation.

The Aspen Plus Data Regression System fits parameters of physical property models to measured data for pure component or multicomponent systems. You can enter almost any kind of experimental property data, such as:

- Vapor-liquid equilibrium
- Liquid-liquid equilibrium
- Density
- Heat capacity
- Activity coefficients

You can use Data Regression for all property models in Aspen Plus, including electrolyte and user models.

This chapter includes the following information about Data Regression:

- Setting up a regression
- Entering pure component, phase equilibrium, and mixture data
- Plotting experimental data
- Formulating a regression case
- Evaluating the accuracy of known model parameters
- Examining and plotting regression results
- Comparing results from several cases
- Using the Dortmund Databank (DDB) interface
- Data regression example

Setting Up a Regression

To set up a Data Regression:

1. Start Aspen Plus and create a new run from a Template as described in Chapter 2.
2. On the New dialog box, select Data Regression in the Run Type list box.

   – or –

   From the Data menu, click Setup. Then choose Data Regression in the Run Type list box on the Setup Specifications Global sheet.
3. Define components on the Components Specifications Selection sheet. See Chapter 6.
4. Select a property method on the Properties Specifications Global sheet. See Chapter 7.
5. Enter or estimate any supplemental property parameters on the Properties Parameters and Properties Estimation forms. See Chapters 9 and 30.
6. Enter experimental data on the Properties Data forms, described later in this chapter.
7. Specify the regression case on the Properties Regression form. See Formulating a Regression Case on page 31-11.

   Use Next to guide you through these steps.

Selecting a Property Method

You must select a property method that uses the property model for which you want to determine parameters.

For example, to fit UNIQUAC binary parameters, choose one of the following property methods:

- UNIQUAC
- UNIQ-HOC
- UNIQ-NTH
- UNIQ-RK

Choose the same property method you will use for simulation runs using the fitted parameters. For example, if you want to use UNIQUAC with the Hayden-O'Connell vapor phase association property method (UNIQ-HOC) in a simulation run, you must also use the UNIQ-HOC property method in your Data Regression run.

There is one important exception. Do not use property methods ending in -2 in Data Regression, even when fitting LLE data. For example, to determine parameters to use with the UNIQ-2 property method, use the UNIQUAC property method in the Data Regression run. In the simulation run, use the UNIQ-2 property method. The binary parameters you determined in the Data Regression run will be available on the Properties Parameters Binary Interaction form.

Entering Supplemental Parameters

If any component being regressed is not in the Aspen Plus databank, do one of the following:

- Enter the required parameters on Properties Parameters forms
- Estimate the parameters using the Properties Estimation forms

For example, suppose you are regressing binary VLE data using the WILSON property method and a component is not in the databank. You must enter or estimate the following parameters: MW, TC, PC, ZC, DHVLWT, PLXANT, and CPIG.

You can also enter values of the parameters to be determined on a Properties Parameters form. Data Regression will use these values as initial guesses.

Fitting Pure Component Data

To fit pure component temperature-dependent property data, such as vapor pressure data:

1. Use the Properties Data PURE-COMP form to enter the experimental data as a function of temperature.
2. Use the Properties Regression Input form to specify the property method, experimental data, and parameters to be regressed.

Entering Pure Component Data

Use the Properties Data PURE-COMP form to enter experimental data for pure component properties as a function of temperature. For example, you can enter vapor pressure versus temperature data.

To enter pure component data:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser, click the Data folder.
3. To create a new Data ID, click New on the Data Object Manager.
4. In the Create New ID dialog box, enter an ID or accept the default. Choose PURE-COMP in the Select Type list box, and click OK.
5. To edit an existing ID, select the Data ID from the Object Manger, and click Edit.
6. On the Setup sheet, select the type of property data in the Property list box. Prompts describe each property. You can limit the types of property data under the Property list box, by selecting a property category in the Category list box. The default category is All.
7. In the Component list box, specify the component for which you have experimental data.
8. In the Temperature and Pressure fields, if active, specify a constant temperature or pressure. A value entered in these fields applies to all data points, and simplifies the entering of isothermal or isobaric data.
9. Click the Data sheet.
10. On the Data sheet, enter the experimental data in the appropriate columns.
11. Enter standard deviation values for the property data or accept the system defaults. See Entering Standard Deviations of Measurements, this chapter.

If you want Aspen Plus to ignore some data or standard deviations that have already been entered, go to the Usage field, click on the row, and select Ignore. Aspen Plus will not use the data point in any subsequent regressions.

Fitting Phase Equilibrium and Mixture Data

To fit phase equilibrium and mixture data, such as vapor-liquid equilibrium and mixture density data:

1. Use the Properties Data MIXTURE form to enter experimental data. See the following section.
2. Use the Properties Regression Input form to specify the property method, experimental data, and the binary or pair parameters to be regressed. See Formulating a Regression Case, this chapter.

Entering Phase Equilibrium and Mixture Data

Use the Properties Data MIXTURE form to enter experimental data for phase equilibrium and mixture properties as a function of temperature, pressure, and composition. For example, you can enter Txy vapor-liquid equilibrium data for two components.

To enter phase equilibrium and mixture data:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser, click the Data folder.
3. To create a new Data ID, click New on the Data Object Manager. In the Create New ID dialog box, enter and ID or accept the default. Choose MIXTURE in the Select Type list box, and click OK.
4. To edit an existing ID, select the Data ID from the Object Manger, and click Edit.
5. On the Setup sheet, choose the type of property data in the Data Type list box, from the choices in Tables 31.1 and 31.2. You can limit the types of property data under the Property list box, by selecting a property category in the Category list box. The default category is All.
6. Select the components from the Available Components list, and use the right arrow button to move them to the Selected Components list.
7. In the Temperature and Pressure fields, if active, specify a constant temperature or pressure. A value entered in these fields applies to all data points.

8. In the Composition Basis list box, specify the basis of the composition data. You can enter composition data as mole fraction, mass fraction, mole percent, or mass percent. Mole fraction is the default.
9. Click the Data sheet.
10. On the Data sheet, enter the experimental data in the appropriate columns.
11. Enter standard deviations for the property data or accept the system defaults. See Entering Standard Deviations of Measurements, this chapter.

If you want Aspen Plus to ignore some data or standard deviations that have already been entered, go to the Usage field, click on the row, and select Ignore. Aspen Plus will not use the data point in any subsequent regressions.

Data Types

Vapor-Liquid Equilibrium Data

Select	For this data
TXY	Isobaric VLE
PXY	Isothermal VLE
TPXY	T-P-x-y VLE
ALPHA	Relative volatility. Defined with respect to the first component listed on the form.

Liquid-Liquid Equilibrium Data[†]

Select	For this data
TXX	T-x-x
PXX	P-x-x
TPXX	T-P-x-x
TPXXY[†]	T-P-x-x-y

[†] *Vapor-liquid-liquid equilibrium data*

[††] *Use with NRTL or UNIQUAC-based property methods; the ELECNRTL property method; or SR-POLAR, PRWS, PRMHV2, RKSWS, RKSMHV2, and PSRK equation-of-state property methods.*

Mixture Property Data

Select	For this data
CPLMX	Liquid heat capacity
CPVMX	Vapor heat capacity
CPSMX	Solid heat capacity

Continued

Mixture Property Data (Continued)

Select	For this data
GLXS	Excess liquid Gibbs free energy
HLMX	Liquid enthalpy
HLXS	Excess liquid enthalpy
HVMX	Vapor enthalpy
HSMX	Solid enthalpy
KLMX	Liquid thermal conductivity
KVMX	Vapor thermal conductivity
KSMX	Solid thermal conductivity
MULMX	Liquid viscosity
MUVMX	Vapor viscosity
RHOLMX	Liquid mass density
RHOVMX	Vapor mass density
RHOSMX	Solid mass density
SIGLMX	Liquid surface tension
USER-X	User property versus x
USER-Y	User property versus y
VLMX	Liquid molar volume
VVMX	Vapor molar volume
VSMX	Solid molar volume

Partial Property Data (Data for Components in a Mixture)

Select	For this data
DLMX	Liquid diffusion coefficients
DVMX	Vapor diffusion coefficients
GAMMA	Liquid activity coefficients
GAMMAS	Solid activity coefficients
HENRY	Henry's constants
KLL	Liquid-liquid distribution coefficients
KVL	Vapor-liquid K-values
USERI-X	User partial property versus x
USERI-Y	User partial property versus y

Data Types for Electrolyte Systems

Select	For this type of data	To
GAMMAM	Mean ionic activity coefficient[†]	Determine parameters for the electrolyte activity coefficient model
HLMX	Liquid molar enthalpy	Determine the temperature dependency of binary or pair parameters for the activity coefficient model[††]
OSMOT	Osmotic coefficient	Determine parameters for the electrolyte activity coefficient model
PH	pH	Determine chemical equilibrium constants (use only the apparent component approach)
TPX	Salt solubility[†††]	Regress parameters for the electrolyte activity coefficient model and chemical equilibrium constants for precipitating salts. Obtain electrolyte-electrolyte pair parameters for the electrolyte NRTL model
TX	Salt solubility[†††]	
TXY, PXY, or TPXY	Vapor liquid equilibrium	Regress electrolyte activity coefficient model parameters, Henry's constants, and chemical equilibrium constants
TXX, TPXX, or TPXXY	Liquid liquid equilibrium	Regress electrolyte activity coefficient model parameters and chemical equilibrium constants
VLMX	Liquid molar volume	Determine parameters for the Clarke density model

[†] *You can enter only the molality scale mean ionic activity coefficient data of single electrolyte systems.*

[††] *Use data at several temperatures to ensure accurate representation of heat of mixing.*

[†††] *Enter at saturation, for single or mixed electrolyte solutions. You must specify the salt precipitation reactions on the Reactions Chemistry form.*

Generating Binary VLE and LLE Data

You can generate VLE and LLE data for a two-component system, using a specified property method. Aspen Plus can then use the generated data to regress parameters for another property method. With this feature you can convert parameters between different property models.

For example, you can generate VLE data using the UNIFAC predictive property method, then use the generated data to determine the binary parameters for the WILSON property method.

To generate binary VLE and LLE data:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser, click the Data folder.
3. To create a new Data ID, click New on the Data Object Manager.
4. In the Create New ID dialog box, enter an ID or accept the default. Choose MIXTURE in the Select Type list box, and click OK.
5. To edit an existing ID, select the Data ID from the Object Manger, and click Edit.
6. On the Setup sheet, choose the type of property data in the Data Type list box:

Select	To generate this data
TXY, PXY, or TPXY	VLE
TXX or TPXX	LLE

   Do not select the GEN-TPXY or GEN_TPXX data type

7. Select the components from the Available Components list and click the right arrow button to move them to the Selected Components list.
8. In the Temperature and Pressure fields, if active, specify a constant temperature or pressure at which the data will be generated.
9. Click the Data sheet.
10. On the Data sheet, click the Generate Data button.
11. In the Generate Binary VLE or LLE Data dialog box, select a property method, and a Henry's Components ID and Chemistry ID, if applicable.
12. Click the Generate button to generate the data.

    The Data sheet displays the liquid phase compositions for which data are to be generated for the regression.

Entering Standard Deviations of Measurements

The standard deviation of a measurement variable is an estimate of the magnitude of random error. Data Regression assigns reasonable default values for standard deviations, based on the property or data type you select. If you know the standard deviations of your data, enter them on the Properties Data Data sheet.

Data Regression assigns the following default standard deviation values:

For	Value
Temperature	0.1 degrees†
Pressure	0.1%
Liquid compositions	0.1%
Vapor compositions	1.0%
Properties	1.0%

† *For Txx or TPxx data, the default is 0.01*

You can assign a set of standard deviation values to:

- A single data point
- Several data points
- All data points in a data group

To enter a standard deviation row on a Properties Data Data sheet, go to the Usage field, and select Std-Dev. The values you enter will apply to all subsequent data points until another Std-Dev row is encountered. Enter the standard deviation in percent or as an absolute value. Data Regression does not require precise values of standard deviations. Usually you only need to determine the appropriate order of magnitude and ratios.

A variable that has a standard deviation value of zero is treated as error-free. Only state variables with little or no random error can have standard deviations of zero. Properties such as vapor pressure or density cannot. You cannot enter all standard deviation values as zero.

For phase equilibrium data, such as TPXY data, the number of non-zero standard deviations must be greater than or equal to the number of phase equilibrium constraints (or equivalently, the number of components in the mixture that participate in phase equilibrium). For example, for TPXY data of two components, you can assign a standard deviation of zero to only two variables. Either T or P, and either X(1) or Y(1) can have zero standard deviations. An exception is TPX data. You can set the standard deviation of X and either T or P to zero.

Unrealistically small standard deviations for "noisy" measurement variables cause convergence problems.

Plotting Experimental Data

You can display a plot of the experimental data you entered using the Plot Wizard from the plot menu.

Depending on the type of data you entered, the Plot Wizard allows the following types:

Plot Typet	Description
T-xy	T-xy plot for isobaric VLE data
P-xy	P-xy plot for isothermal VLE data
T-x	T-x plot for isobaric VLE data
P-x	P-x plot for isothermal VLE data
y-x	y-x plot for VLE data
T-xx	T-xx plot for LLE data
P-xx	P-xx plot for LLE data
Prop-x	Property vs. Composition
Prop-T	Property vs. Temperature
Triangular	Triangular diagram for ternary LLE data

Formulating a Regression Case

Use the Properties Regression forms to formulate a regression case.

A regression case requires:

- Experimental data
- Parameters for regression

To formulate a regression case:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser, click the Regression folder.
3. To create a new Regression ID, click New on the Regression Object Manager. In the Create New ID dialog box, enter an ID or accept the default, and click OK.
4. To edit an existing ID, select the Regression ID from the Object Manger, and click Edit.

5. In the Property Options frame of the Regression Input Setup sheet, specify property method, Henry Components ID, Chemistry ID, and electrolyte calculation method. The global properties specifications you entered on the Properties Specifications Global sheet are the default. You can select any property method already entered on the Properties Specifications form.
6. At the bottom of the Setup sheet, use the Data Set list boxes to enter the Data set IDs for the experimental data to be regressed. To assign more weight to data sets, enter a value greater than 1 in the Weight field.
7. For each Binary VLE Data set referenced, you can choose whether you want a thermodynamic consistency test performed, using the Perform Test check box. If you choose to perform a consistency test, you can use the Test Method list box to choose the type of consistency test. Also select whether you want to reject data sets that fail the consistency test, using the Reject check box. For more information see Thermodynamic Consistency Test for VLE Data, this chapter.
8. Click the Parameters sheet.
9. Enter the Parameters to be regressed, according to the procedure in the following section, Specifying Parameters to be Regressed.

In many cases Aspen Plus will automatically complete the Regression Input form based on the property method and Data sets you have specified. For example, suppose you select the NRTL property method and enter Txy data for a binary system. Aspen Plus completes the Regression Input form by:

- Filling in the Data ID field
- Specifying that the NRTL binary parameters are to be regressed

Specifying Parameters to be Regressed

In cases where the parameters to be regressed are not specified automatically, or when you want to modify the default parameters or add additional parameters, you can use the Regression Input Parameters sheet.

To specify parameters to be regressed:

1. In the Type field of the Regression Input Parameters sheet, select one:

Option	For
Parameter	Pure component parameter
Binary parameter	Binary parameter
Group parameter	UNIFAC group parameter
Group binary parameter	UNIFAC group binary parameter
Pair parameter	Electrolyte NRTL model pair parameter
Chemistry	Equilibrium constants for electrolyte chemistry

2. In the Name/Element list box, select the parameter names. The prompt identifies parameters.
3. Enter the element number of the parameter in the field just to the right of the parameter name. For group interaction parameters for the Lyngby-modified UNIFAC and the Dortmund-modified UNIFAC models, only the first element can be regressed.
4. Enter the component(s) or UNIFAC group IDs in the Component/Group list boxes.
5. For each parameter, use the Usage list box to:

Specify	**If you want the parameter to be**
Regress†	Used in the current regression case
Exclude	Excluded from the current regression case.†† The value in the Initial Value field is ignored.
Fix	Set to the fixed value given in the Initial Value field†††

† *Default*

†† *If the parameter is in the databank or has been entered on the Properties Parameters forms, Aspen Plus uses this value in the property calculation during the regression.*

††† *You can fix a parameter to a given value in one case, then set it to another value in another case to study the effect on the fit. For example, you can fix the third element of the NRTL binary parameter (the nonrandomness factor) in a case study to see which value gives the best results.*

6. You can enter Initial Value, Lower Bound, Upper Bound, and Scale Factor for the parameter.

Thermodynamic Consistency Test for VLE Data

Aspen Plus tests the binary VLE data you enter on the Data Mixture form for thermodynamic consistency when you supply both of the following:

- Composition data for both the liquid and vapor phases
- At least five data points, not counting pure component data points (x=0.0 and x=1.0)

Aspen Plus provides two methods for testing consistency:

- The area test of Redlich-Kister
- The point test of Van Ness and Fredenslund

Both methods use the Gibbs-Duhem equation. For detailed information on both tests, see J. Gmehling and U. Onken, Vapor-Liquid Equilibrium Data Collection, DECHEMA Chemistry Data Series, Vol. I, Part 1, ed. Dieter Behrens and Reiner Eckermann (Frankfurt/Main: DECHEMA, Deutsche Gesellschaft fur Chemisches Apparatewesen, 1977).

By default, Aspen Plus performs the area test. To select another test method or to change the test tolerance, use the Regression Input Setup sheet. On the Setup sheet you can also specify whether you want to use or reject the data sets that fail the consistency tests.

The Consistency Tests sheet on the Regression Results form indicates whether your data passes or fails the consistency test. Failed data can cause accuracy and convergence problems in your simulation. The test can fail because:

- The data contains errors, either in the original data or occurring during data entry
- The vapor phase equation-of-state model does not appropriately account for the vapor phase nonideality
- You do not have enough data points or the data cover only a small concentration range. To obtain meaningful consistency test results, enter data for the entire valid composition range.

If your data fail the test, check the data values and units in the Txy, Pxy, or TPxy data you entered on the Data Mixture form.

To obtain meaningful consistency test results, enter data for the entire valid composition range. You can ignore the test results if your data covers only a narrow composition range.

Evaluating the Accuracy of Known Model Parameters

You can use Data Regression to evaluate the accuracy of known model parameters. Compare the calculated results obtained using the model with your experimental data.

1. Select a property method on the Properties Specifications Global sheet. See Chapter 7.
2. Enter the experimental data on the Properties Data forms. See Entering Pure Component Data, and Entering Phase Equilibrium and Mixture Data, this chapter.

3. Enter the known model parameters on the Properties Parameters forms. See Chapter 8. To evaluate parameters stored in the databanks, skip this step.
4. Specify the property method and experimental data to be used in the evaluation on the Regression Input Setup sheet. See Formulating a Regression Case, this chapter.
5. In the Calculation Type frame on the Regression Input Setup sheet, select Evaluation.

Running the Regression

To run the regression, select Run from the Run menu or the Control Panel. If you have more than one regression case, the Data Regression Run Selection dialog box appears. All cases are listed in the Run area. The Don't Run area is empty. You can:

- Run all the cases by clicking on OK.
- Change the order in which the cases are executed. Select a case and use the Up and Down arrows.
- Exclude certain Regression cases from the run. Select a case, then use the left arrow to move the case into the Don't Run area.

The order in which the regression cases are run may be significant. The regressed parameter values from a regression case are used automatically in all subsequent regression cases. Aspen Plus will execute the regression cases in the order they appear in the Run area.

Using Regression Results

This section discusses examining, plotting and comparing regression results.

Examining Regression Results

To examine regression results:

1. From the Data menu, click Properties.
2. In the left pane of the Data Browser, double-click the Regression folder.

3. From the Data Browser menu tree, double-click the Regression ID of interest, and select Results.

   The Regression Results form appears, containing these sheets:

Sheet	Shows
Parameters	Final parameter estimates, final parameter standard deviations, number of iterations and the property method used
Consistency Tests	Thermodynamic consistency test results
Residual	Residual for each property: the experimental value; regressed value; standard deviation; difference between the experimental and regressed values; the percent difference. A summary of the deviation, including average and maximum deviations can be obtaining by clicking the Deviations button
Profiles	All experimental and calculated values. These data are used on all pre-defined plots. (see Plotting Regression Results this chapter)
Correlation	Parameter correlation matrix: intercorrelation between the parameters
Sum of Squares	Objective function, regression algorithm, initialization method, final weighted sum of squares and residual root mean square error
Evaluation	Property method, final weighted sum of squares and residual root mean square error for the evaluation of experimental data. This result sheet is only active for Evaluation cases.
Extra Property	Residuals for extra properties when VLE data is used, as requested on the Regression Input Report sheet (for example, activity coefficients and K-values)

Problems with Data Regression Results

If your Data Regression run fails to converge, the Properties Data forms probably contain data entry errors. Check the data values and units. Plot the data to check for errors or outliers using the Plot Wizard from the Plot menu.

Inappropriate standards deviations may have been used for the data. See Entering Standard Deviations of Measurements on page 9, for guidelines.

If you use binary VLE data, the data may not be thermodynamically consistent. Request consistency test on the Setup sheet. Rerun the regression. Examine the test results on the Regression Results Consistency Tests sheet.

When fitting different models to the same data set, choose the model that gives the smallest residual root mean square error value.

On the Regression Results Correlation sheet, the off-diagonal elements of the matrix indicate the degree of correlation between any two parameters. When the parameters are completely independent, the correlation coefficient is zero. A number close to 1.0 or -1.0 indicates a high degree of correlation. If possible, select parameters that are not correlated. An important exception: asymmetric binary parameters for activity coefficient models are highly correlated. Both the ij and ji parameters are required for best fits.

How to Identify Unsatisfactory Data Regression Results

It is possible for your Data Regression run to converge without errors, but with results unsuitable for use in a simulation run. Use these Regression Results sheets to identify bad fits:

- Parameters
- Sum of Squares
- Consistency Tests

These signs indicate a bad fit:

- A standard deviation for a regressed parameter is 0.0, indicating the parameter is at a bound.
- A large residual root mean square error value. Normally, this value should be less than 10 for VLE data and less than 100 for LLE data.
- Your VLE data fail the thermodynamic consistency test.

If any of these conditions exist, check the original data source and the data and units on the Properties Data forms for errors. Plot the data using the Plot Wizard from the Plot menu. Use the Regression Results Residual sheet to see how well each data point was fitted. Look for out-liers.

Plotting Regression Results

When viewing the Regression Results form, you can use the Plot Wizard to generate useful plots of the regression results. Aspen Plus provides a number of predefined plots.

To start the Plot Wizard, choose Plot Wizard from the Plot menu on the main menu bar while viewing the Regression Results form. Depending on your type of regression, some of the plots below will be available:

Name of Plot	Description
T-xy	Temperature versus liquid and vapor composition for isobaric VLE data
P-xy	Pressure versus liquid and vapor composition for isobaric VLE data
T-x	Temperature versus liquid composition for isobaric VLE data
P-x	Pressure versus liquid composition for isobaric VLE data
y-x	Vapor versus liquid composition
T-xx	Temperature versus liquid 1 and liquid 2 composition for LLE data
P-xx	Pressure versus liquid 1 and liquid 2 composition for LLE data
Prop-x	Property versus liquid composition
Prop-T	Property versus temperature

Continued

Name of Plot	Description
(y-x) vs. x	Vapor minus liquid composition versus liquid composition
Triangular	Triangular diagram for ternary LLE data
Exp vs. Est	Experimental versus calculated
Residual	Residual versus property

The residual versus property plot shows how the errors are distributed. If the measurement data contain no systematic errors, the deviations should distribute randomly around the zero axis.

Predefined plots such as T-xy or P-xy display the experimental data as symbols and the calculated values as lines. These plots allow you to assess the quality of the fit. You can also identify bad data points by comparing the experimental data with the calculated results.

You can use the Property Analysis capabilities (see Chapter 29) to plot T-xy or P-xy diagrams at other conditions to check the extrapolation of the regressed parameters.

Comparing Results from Several Cases

You can plot the results from several Regression cases on a single plot. This allows you to compare several property models in fitting the same sets of data. To plot results from several cases, select Add to Plot on the Plot Wizard (step 3). For example, you could make a Txy plot using results from two cases:

1. From the Plot menu of a results form of the first case, use the Plot Wizard to generate a T-xy plot.
2. Select the data group and component to plot. Click Next or Finish to display the plot
3. Go to the Regression Results form. Do not close the plot.
4. Use the Plot Wizard from the Plot menu. Select the T-xy plot type. Click Next
5. Select the same data group and component as in step 2
6. For select Plot Mode, select Add to Plot, then select the first plot from the list box
7. Click Next of Finish to display the combined plot.

You can change the plot attributes as necessary, by using the Properties option from the right mouse button menu.

Using Regression Results in a Flowsheet Run

The parameters determined by regression are placed automatically on the appropriate Properties Parameters forms. To use the regressed parameters in a flowsheet run:

1. From the Data Browser, select the Setup Specifications Global sheet.
2. In the Run-type field, select Flowsheet.

You can copy regression and estimation results onto parameters forms on the Component Data sheet:

1. From the Tools menu, select Options.
2. Click the Component Data tab.
3. Check the Copy Regression and Estimation Results Onto Parameters Forms check box.

Retrieving Data From DETHERM and the Internet

You can retrieve a wide range of experimental data from DETHERM and the internet. DETHERM contains the world's most comprehensive collection of thermo physical property and phase equilibrium data. If you have a valid license to use DETHERM, click the DETHERM icon on the main application tool bar to search for the experimental data you need. Experimental data you retrieve will appear on the Properties Data forms and are ready for use in data regression. Please call your account manger at Aspen Technology to register to use Internet DETHERM.

Example of Regressing Vapor Liquid Equilibrium Data for Ethanol and Ethyl-Acetate

For an ethanol-ethyl acetate system, the following vapor liquid equilibrium data are available.

40C and 70C data of Martl, *Collect. Czech. Chem. Commun.* 37,266 (1972):

T=40C

P MMHG	X ETOAC	Y ETOAC
136.600	0.00600	0.02200
150.900	0.04400	0.14400
163.100	0.08400	0.22700
183.000	0.18700	0.37000
191.900	0.24200	0.42800
199.700	0.32000	0.48400
208.300	0.45400	0.56000
210.200	0.49500	0.57400
211.800	0.55200	0.60700
213.200	0.66300	0.66400
212.100	0.74900	0.71600
204.600	0.88500	0.82900
200.600	0.92000	0.87100
195.300	0.96000	0.92800

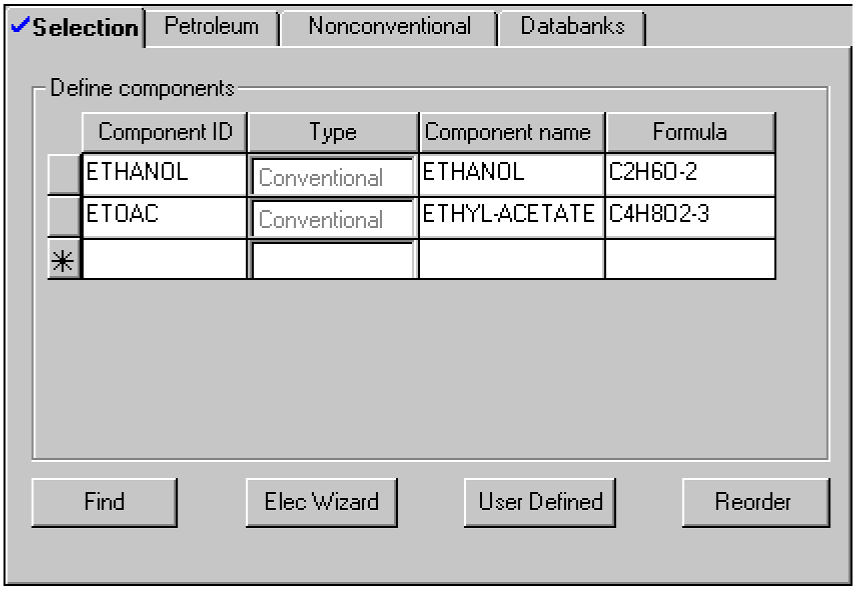
T=70C

P MMHG	X ETOAC	Y ETOAC
548.600	0.00650	0.01750
559.400	0.01800	0.04600
633.600	0.13100	0.23700
664.600	0.21000	0.32100
680.400	0.26300	0.36700
703.800	0.38700	0.45400
710.000	0.45200	0.49300
712.200	0.48800	0.51700
711.200	0.62500	0.59700
706.400	0.69100	0.64100
697.800	0.75500	0.68100
679.200	0.82200	0.74700
651.600	0.90300	0.83900
635.400	0.93200	0.88800
615.600	0.97500	0.94800

Atmospheric data of Ortega J. and Pena J.A., *J. Chem. Eng. Data* 31, 339 (1986):

T C	X ETOAC	Y ETOAC	T C	X ETOAC	Y ETOAC
78.450	0.00000	0.00000	71.850	0.44700	0.48700
77.400	0.02480	0.05770	71.800	0.46510	0.49340
77.200	0.03080	0.07060	71.750	0.47550	0.49950
76.800	0.04680	0.10070	71.700	0.51000	0.51090
76.600	0.05350	0.11140	71.700	0.56690	0.53120
76.400	0.06150	0.12450	71.750	0.59650	0.54520
76.200	0.06910	0.13910	71.800	0.62110	0.56520
76.100	0.07340	0.14470	71.900	0.64250	0.58310
75.900	0.08480	0.16330	72.000	0.66950	0.60400
75.600	0.10050	0.18680	72.100	0.68540	0.61690
75.400	0.10930	0.19710	72.300	0.71920	0.64750
75.100	0.12160	0.21380	72.500	0.74510	0.67250
75.000	0.12910	0.22340	72.800	0.77670	0.70200
74.800	0.14370	0.24020	73.000	0.79730	0.72270
74.700	0.14680	0.24470	73.200	0.81940	0.74490
74.500	0.16060	0.26200	73.500	0.83980	0.76610
74.300	0.16880	0.27120	73.700	0.85030	0.77730
74.200	0.17410	0.27800	73.900	0.86340	0.79140
74.100	0.17960	0.28360	74.100	0.87900	0.80740
74.000	0.19920	0.30360	74.300	0.89160	0.82160
73.800	0.20980	0.31430	74.700	0.91540	0.85040
73.700	0.21880	0.32340	75.100	0.93670	0.87980
73.300	0.24970	0.35170	75.300	0.94450	0.89190
73.000	0.27860	0.37810	75.500	0.95260	0.90380
72.700	0.30860	0.40020	75.700	0.96340	0.92080
72.400	0.33770	0.42210	76.000	0.97480	0.93480
72.300	0.35540	0.43310	76.200	0.98430	0.95260
72.000	0.40190	0.46110	76.400	0.99030	0.96860
71.950	0.41840	0.46910	77.150	1.00000	1.00000
71.900	0.42440	0.47300			

1. Start Aspen Plus and create a new run, selecting Data Regression as the Run Type.
2. Enter the components on the Components Specifications Selection sheet:



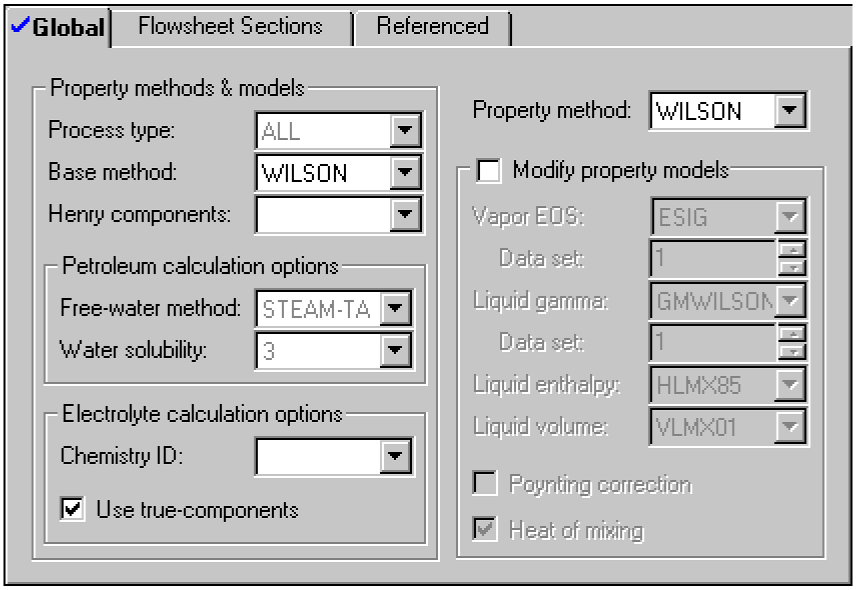
Component ID	Type	Component name	Formula
ETHANOL	Conventional	ETHANOL	C2H6O-2
ETOAC	Conventional	ETHYL-ACETATE	C4H8O2-3

Note A complete backup file with results for this example is available in the Aspen Plus Online Applications Library. The filename is DRS1.

In this example three activity coefficient models will be fitted to the VLE data, each in a separate case.

3. Select the property method.

   Use the Properties Specifications Global sheet to choose a property method. This example compares fitting results for the Wilson, NRTL, and UNIQUAC property methods. Select one of the three on the Global sheet and the remaining two on the Referenced sheet. In this example, the Wilson model is chosen on the Global sheet.

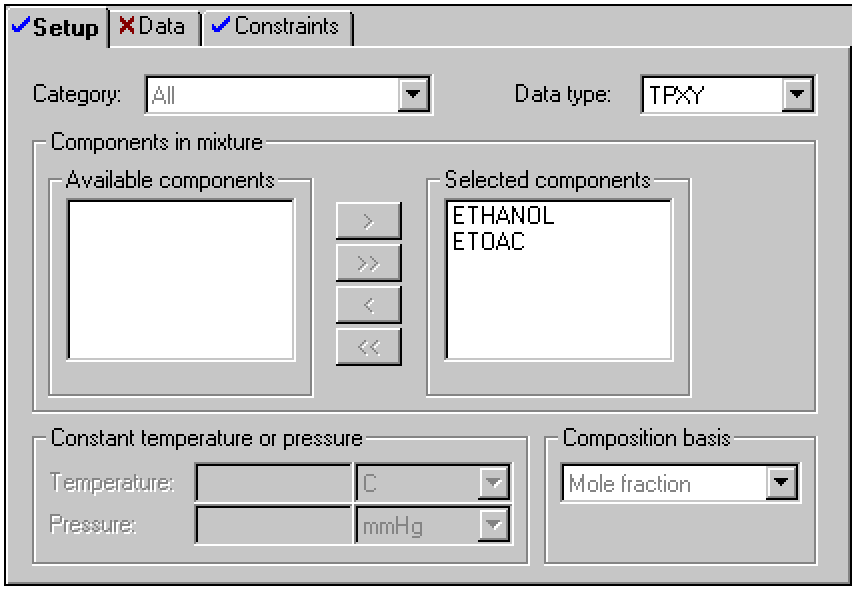


Property methods & models
Process type: ALL
Base method: WILSON
Henry components:
Petroleum calculation options
Free-water method: STEAM-TA
Water solubility: 3
Electrolyte calculation options
Chemistry ID:
☑ Use true-components

Property method: WILSON
☐ Modify property models
Vapor EOS: ESIG
Data set: 1
Liquid gamma: GMWILSON
Data set: 1
Liquid enthalpy: HLMX85
Liquid volume: VLMX01
☐ Poynting correction
☑ Heat of mixing

4. Enter experimental data.

   Use the Properties Data Mixture form to enter the vapor liquid equilibrium data. Three data sets are required, one for each set of VLE data. The following setup and Data sheets are for the 40°C isothermal data set.

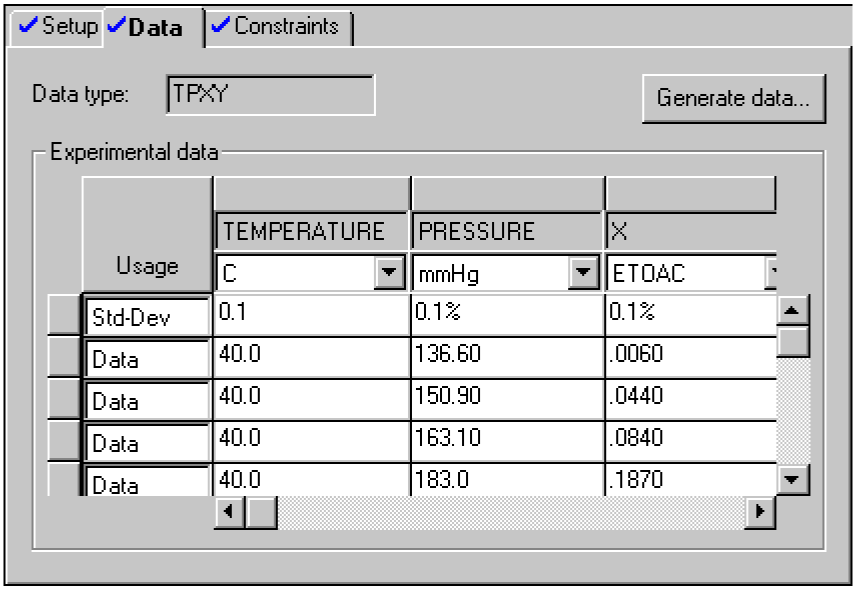


Category: All

Data type: TPXY

Selected components:
ETHANOL
ETOAC

Composition basis: Mole fraction

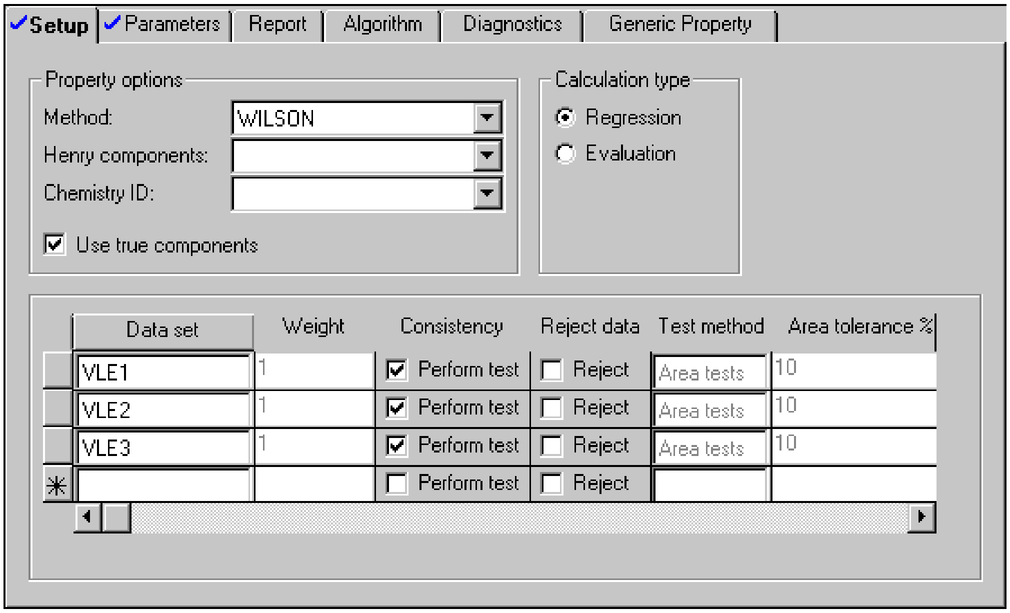


Data type: TPXY

Usage	TEMPERATURE	PRESSURE	X
	C	mmHg	ETOAC
Std-Dev	0.1	0.1%	0.1%
Data	40.0	136.60	.0060
Data	40.0	150.90	.0440
Data	40.0	163.10	.0840
Data	40.0	183.0	.1870

5. Specify the regression case.

   Use the Properties Regression form to formulate a regression case. In this example, Aspen Plus has already completed the Properties Regression Input form. Since the WILSON property method is the Global property method, it is used as the default in the regression. All the VLE data groups you entered in Step 4 are on this form. Aspen Plus will test the data for thermodynamic consistency, using the Area test.



Property options

Method: WILSON

Henry components:

Chemistry ID:

☑ Use true components

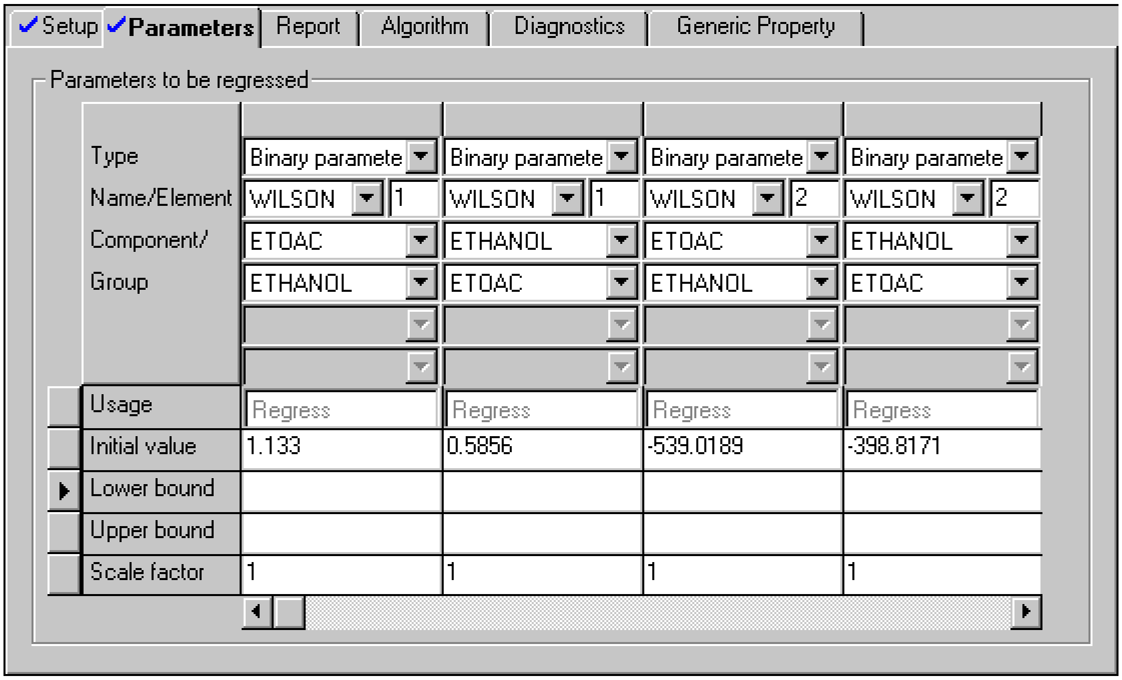
Calculation type

● Regression

○ Evaluation

Data set	Weight	Consistency	Reject data	Test method	Area tolerance %
VLE1	1	☑ Perform test	☐ Reject	Area tests	10
VLE2	1	☑ Perform test	☐ Reject	Area tests	10
VLE3	1	☑ Perform test	☐ Reject	Area tests	10
*		☐ Perform test	☐ Reject		

Since the VLE data cover a wide temperature range, Aspen Plus selects elements 1 and 2 of the Wilson binary parameters for regression. Aspen Plus uses the databank values for the binary parameters as initial guesses in the regression.

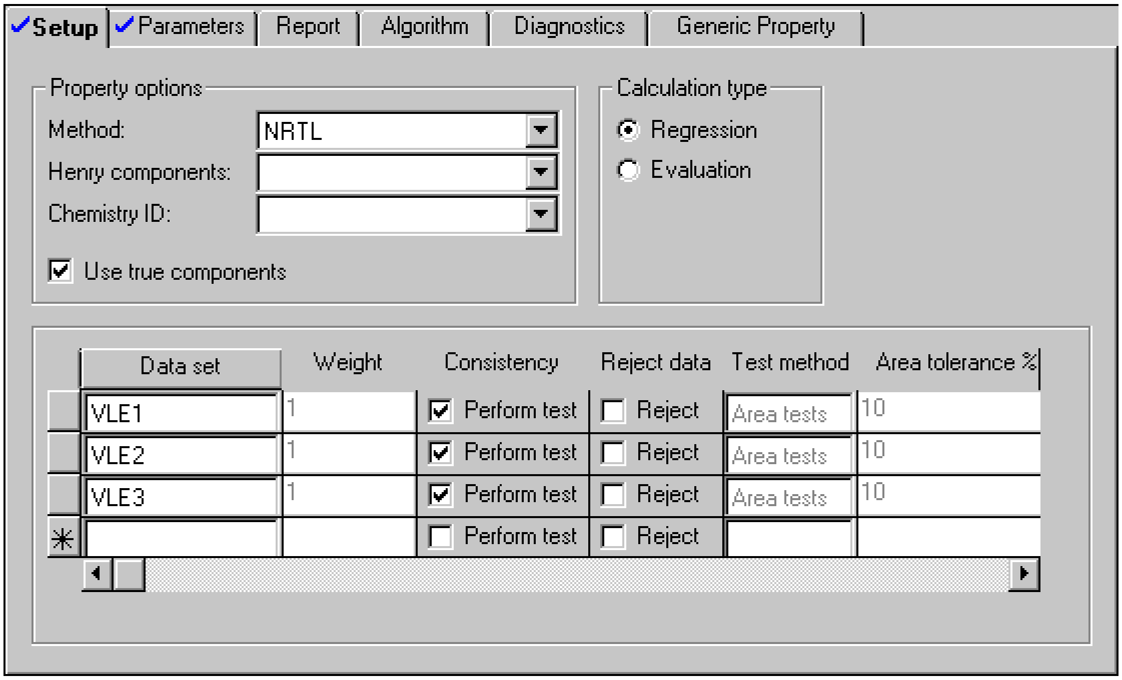


Parameters to be regressed

Type	Binary paramete	Binary paramete	Binary paramete	Binary paramete
Name/Element	WILSON 1	WILSON 1	WILSON 2	WILSON 2
Component/ Group	ETOAC ETHANOL	ETHANOL ETOAC	ETOAC ETHANOL	ETHANOL ETOAC
Usage	Regress	Regress	Regress	Regress
Initial value	1.133	0.5856	-539.0189	-398.8171
Lower bound				
Upper bound				
Scale factor	1	1	1	1

6. Specify additional regression cases.

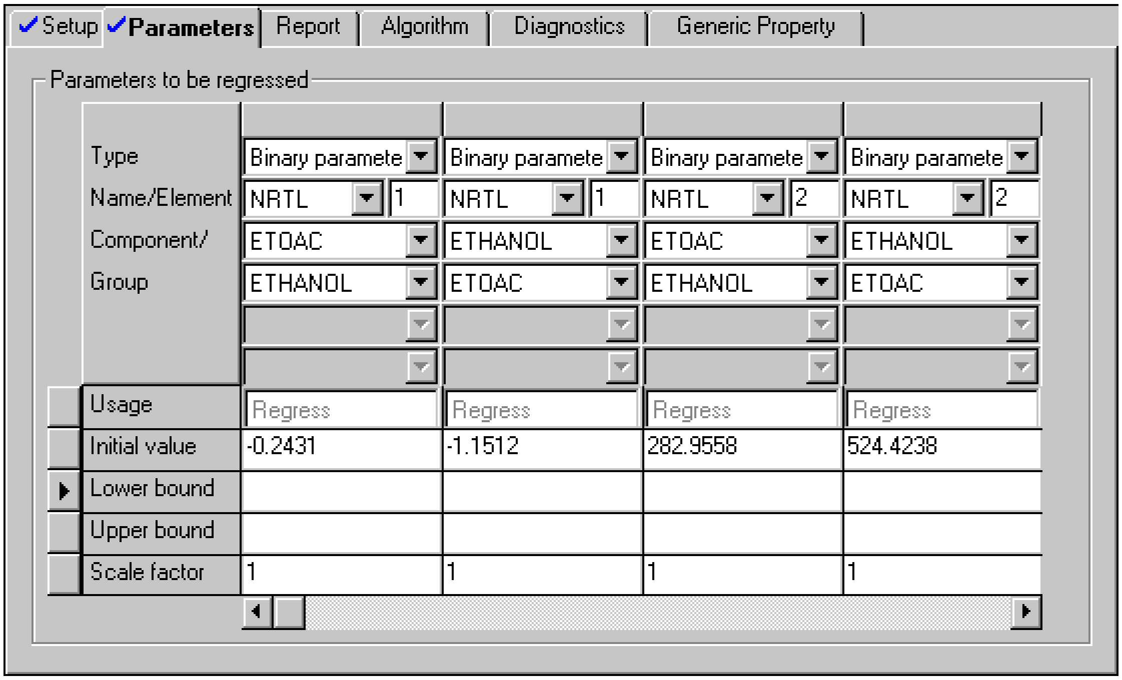
Use the Regression Object Manager to specify two additional cases. Use the same set of experimental data, but with the NRTL and UNIQUAC property methods. Again Aspen Plus completes the Regression Input form. However, since the WILSON property method is the global property method , it is the default. Specify NRTL in the Method list box on the Setup sheet, so that the NRTL property method is used in the second case. When the NRTL property method is used, the NRTL binary parameters must be regressed. Specify the NRTL binary parameter elements 1 and 2 as the regression parameters.



Property options
Method: NRTL
Henry components:
Chemistry ID:
☑ Use true components

Calculation type
● Regression
○ Evaluation

Data set	Weight	Consistency	Reject data	Test method	Area tolerance %
VLE1	1	☑ Perform test	☐ Reject	Area tests	10
VLE2	1	☑ Perform test	☐ Reject	Area tests	10
VLE3	1	☑ Perform test	☐ Reject	Area tests	10
		☐ Perform test	☐ Reject		

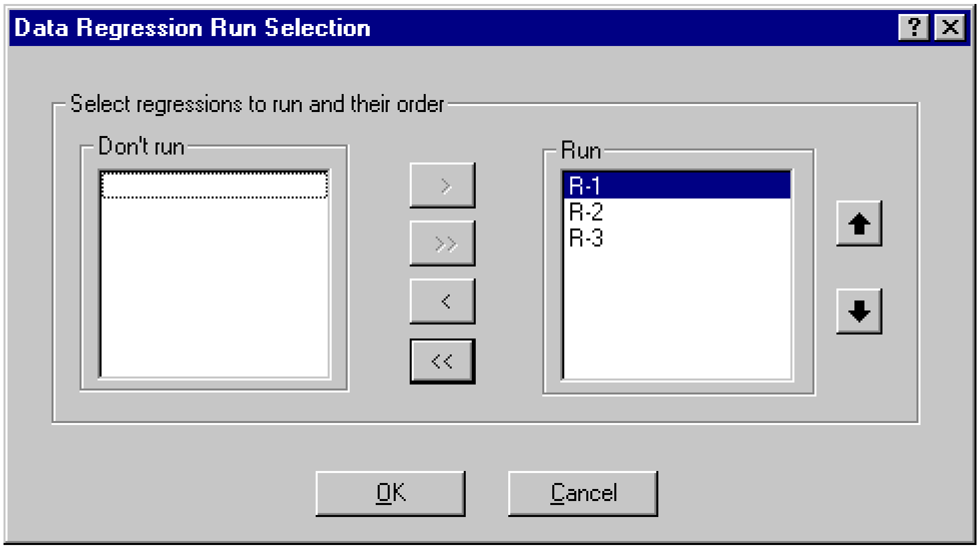


Type	Binary paramete	Binary paramete	Binary paramete	Binary paramete
Name/Element	NRTL 1	NRTL 1	NRTL 2	NRTL 2
Component/	ETOAC	ETHANOL	ETOAC	ETHANOL
Group	ETHANOL	ETOAC	ETHANOL	ETOAC
Usage	Regress	Regress	Regress	Regress
Initial value	-0.2431	-1.1512	282.9558	524.4238
Lower bound				
Upper bound				
Scale factor	1	1	1	1

Repeat this step for the UNIQUAC property method.

7. Run the regression.

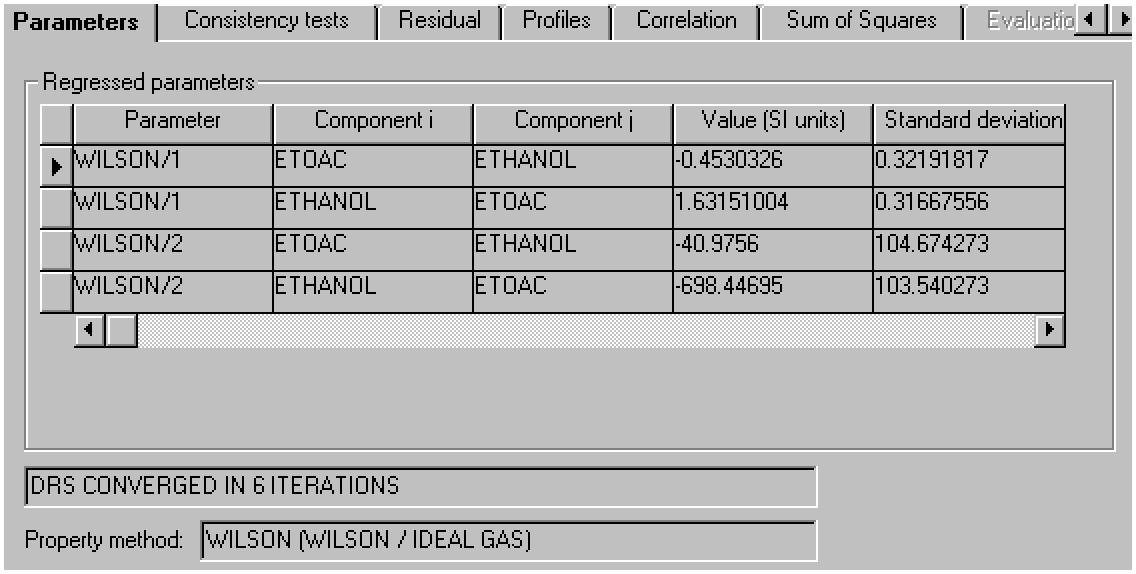
Run all three cases. Click OK on the Data Regression Run Selection dialog box. You can also run selected cases. Move the cases you do not want to run into the Don't Run area, using the left arrow.



Run:
R-1
R-2
R-3

8. Examine the results on the Regression Results form.

Use the Regression Results Parameters sheet to examine the final parameter values.



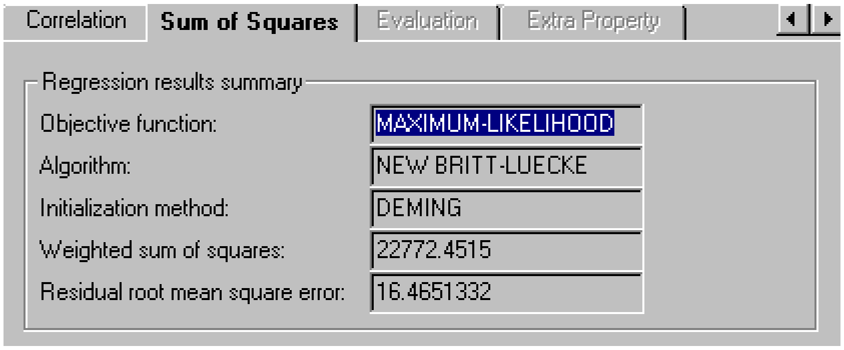
Regressed parameters

Parameter	Component i	Component j	Value (SI units)	Standard deviation
WILSON/1	ETOAC	ETHANOL	-0.4530326	0.32191817
WILSON/1	ETHANOL	ETOAC	1.63151004	0.31667556
WILSON/2	ETOAC	ETHANOL	-40.9756	104.674273
WILSON/2	ETHANOL	ETOAC	-698.44695	103.540273

DRS CONVERGED IN 6 ITERATIONS

Property method: WILSON (WILSON / IDEAL GAS)

Use the Regression Results Sum of Squares sheet to examine the weighted sum of squares and residual root mean square errors.

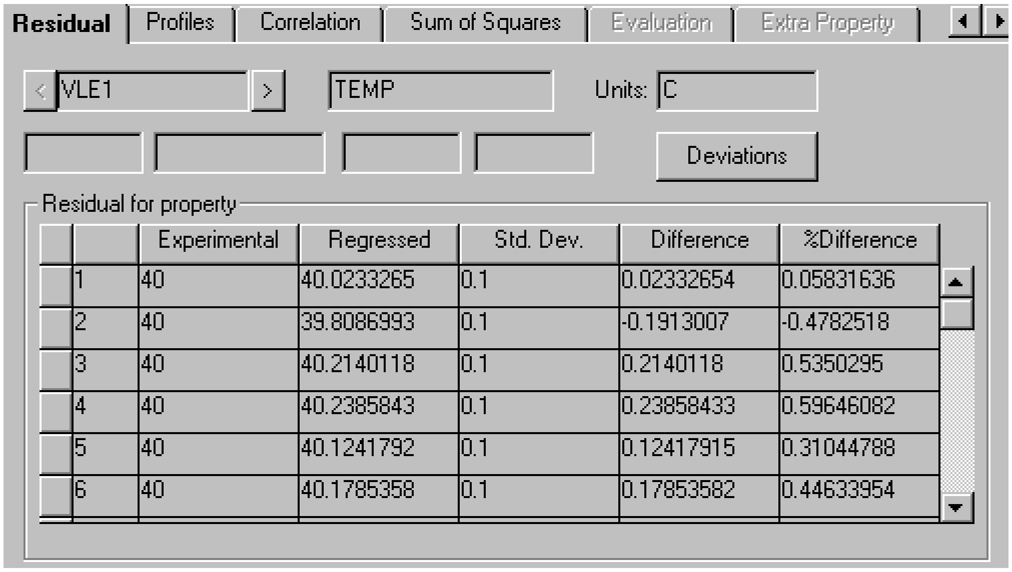


Regression results summary

Objective function: MAXIMUM-LIKELIHOOD
Algorithm: NEW BRITT-LUECKE
Initialization method: DEMING
Weighted sum of squares: 22772.4515
Residual root mean square error: 16.4651332

Use the Regression Results Consistency Tests sheet to examine the results of thermodynamic consistency tests. All data groups passed the Redlich Kister area test.

Use the Regression Results Residual sheet to examine the residual for the fit of pressure, temperature, and composition.

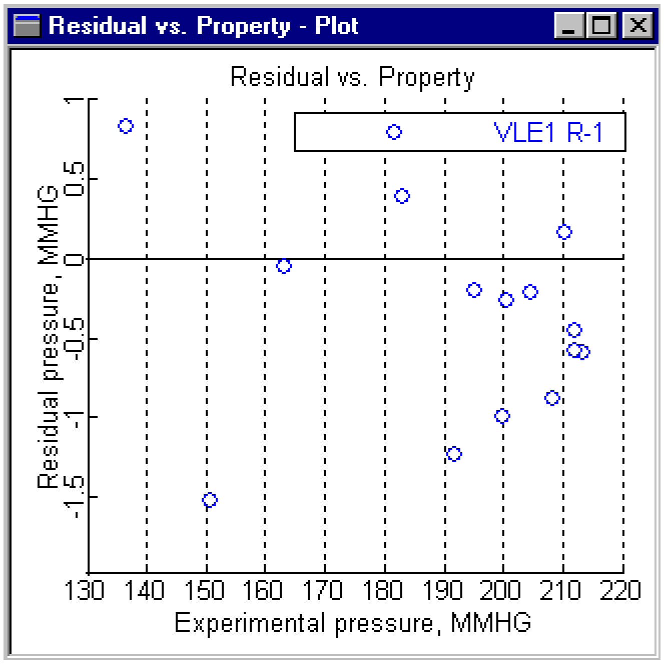


VLE1 TEMP Units: C

Residual for property

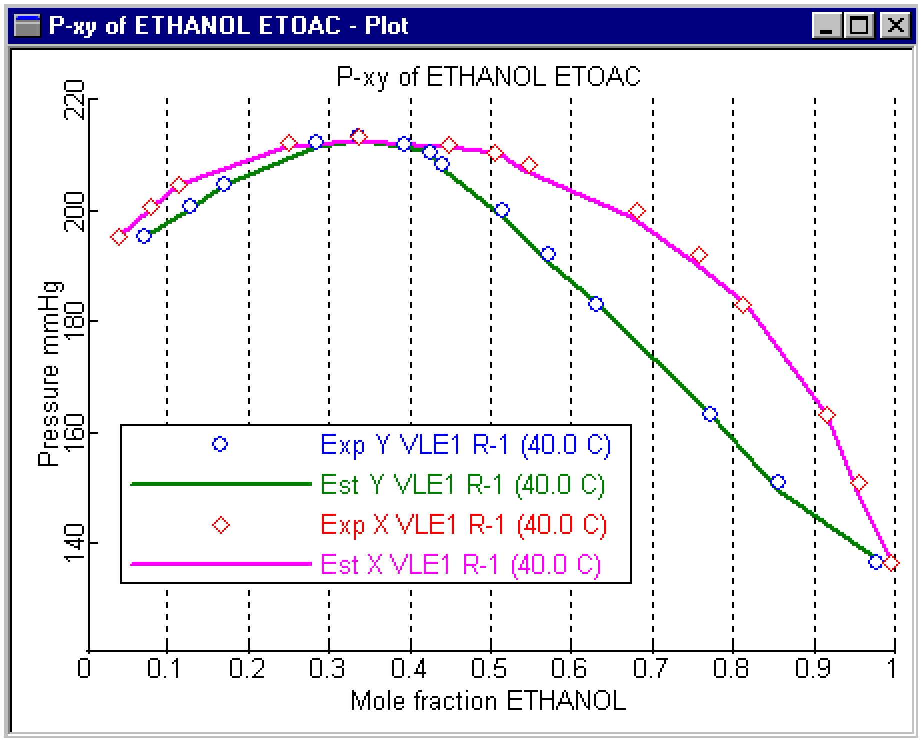
		Experimental	Regressed	Std. Dev.	Difference	%Difference
	1	40	40.0233265	0.1	0.02332654	0.05831636
	2	40	39.8086993	0.1	-0.1913007	-0.4782518
	3	40	40.2140118	0.1	0.2140118	0.5350295
	4	40	40.2385843	0.1	0.23858433	0.59646082
	5	40	40.1241792	0.1	0.12417915	0.31044788
	6	40	40.1785358	0.1	0.17853582	0.44633954

Use Plot Wizard from the Plot menu to plot the residual of pressure for case VLE 1.



You can also plot the residual of other variables.

It is most useful to compare experimental data with calculated results. From the Plot menu, use the Plot Wizard to generate a P-xy plot for the first data group.



Add the results from the NRTL and UNIQUAC cases to the plot for WILSON. (See Comparing Results From Several Cases, this chapter.)

❖ ❖ ❖ ❖

32

Petroleum Assays and Pseudocomponents

This chapter explains how to use the Assay Data Analysis and Pseudocomponent System (ADA/PCS) to define and characterize petroleum mixtures.

Topics include how to:

- Use ADA/PCS
- Create assays and enter assay data
- Create a blend and enter blend specifications
- Generate and define pseudocomponents
- Define and modify petroleum properties
- Examine ADA/PCS results

About ADA/PCS

You can use ADA/PCS for defining and characterizing petroleum mixtures.

You can enter data for any number of assays. The minimum assay data consists of a distillation curve and a bulk gravity value. You can enter optional data, such as:

- Light-ends analysis
- Gravity curve
- Molecular weight curve

You can enter any number of petroleum property curves, such as:

- Sulfur content
- Metal content
- Freeze point

- Octane numbers

Given data for any number of assays, ADA/PCS:

- Converts the distillation data into the true boiling point basis
- Performs extrapolations on assay curves and estimates any missing data
- Generates blends from two or more assays
- Develops sets of pseudocomponents to represent the assays and blends
- Reports distillation curves for assays and blends in user-specified bases
- Estimates physical properties for each pseudocomponent

You can define your own pseudocomponents and use ADA/PCS to estimate their physical properties.

Using ADA/PCS

You can use ADA/PCS in:

- A standalone Assay Data Analysis run
- A Flowsheet simulation run

To use ADA/PCS on a standalone basis, specify Assay Data Analysis in the Run Type list on the Setup Specifications Global sheet. Or specify Assay Data Analysis in the Run Type list on the New dialog box when creating a new run.

In an Assay Data Analysis run, only ADA/PCS calculations are performed. You can display and plot the distillation curves for assays and blends in different bases, and examine the generated pseudocomponents and their properties.

In a Flowsheet run, you can use assays, blends, and pseudocomponents to define process feed streams for the simulation. If you entered petroleum properties, Aspen Plus automatically associates these properties with the streams.

Creating Assays

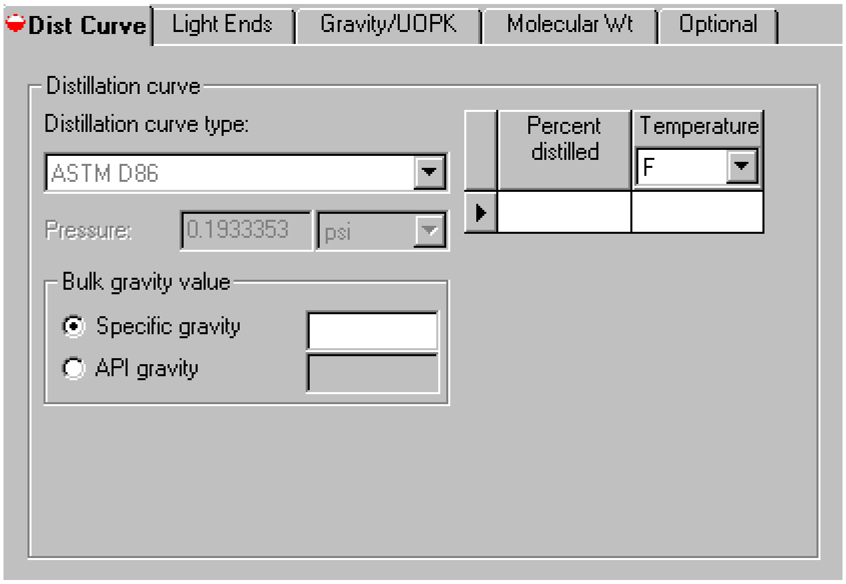
You can define an assay using one of the following:

- Components Specifications Selection sheet
- Assay-Blend Object Manager

Defining an Assay Using the Components Specifications Selection Sheet

To define an assay using the Components Specifications Selection sheet:

1. From the Data menu, select Components, then Specifications.
2. On the Components Specifications Selection sheet, enter a name for the assay in the Component ID field.
3. In the Type list, select Assay as the component type.
4. In the left pane of the Data Browser, click the Assay/Blend folder.
5. In the Assay/Blend Object Manager, select the Assay ID for which you are entering assays, then click Edit. The Components Assay/Blend Basic Data form appears:



Distillation curve type: ASTM D86

Pressure: 0.1933353 psi

● Specific gravity

○ API gravity

Temperature: F

Select the appropriate Assay sheet to enter assay data.

Defining an Assay Using the Assay-Blend Object Manager

To define an assay using the Assay-Blend Object Manager:

1. From the Data menu, select Components, then Assay/Blend.
2. On the Assay-Blend Object Manager, click New.
3. In the Create New ID dialog box, choose Assay in the Select Type list.

4. Enter an ID for the assay, or accept the default ID.
5. Click OK.

The Assay Input Menu appears. Select the appropriate Assay sheet to enter assay data.

Entering Assay Data

For each assay you must enter:

- At least four points on a distillation curve
- Either a bulk gravity or a gravity curve

Instructions for enter this required data, as well as other optional data, are contained in the subsequent discussions of sheets and forms.

Entering a Distillation Curve and Bulk Gravity Value

The assay distillation curve and bulk gravity value are entered on the Dist Curve sheet of the Components Assay/Blend Basic Data form.

To enter the required distillation curve and gravity input:

1. From the Data menu, select Components, then Assay/Blend.
2. On the Assay-Blend Object Manager, select the assay for which you wish to enter data, and click Edit.
3. On the Dist Curve sheet, select a type of curve in the Distillation Curve Type list.
4. In the Percent Distilled and Temperature columns, enter at least four pairs of distillation percent and temperature values for the curve.
5. In the Bulk Gravity Value frame, enter either Specific Gravity or API Gravity, by clicking the appropriate radio button, and typing in the value.

   - or -

   Click the Gravity/UOPK tab to open that sheet, and enter in a gravity curve. (See next section for details on entering a gravity curve.)

   By default Aspen Plus reports the distillation curve in the input and the true boiling (liquid volume) basis. You can use the Optional sheet to request additional distillation curves to be reported for the assay.

Use the remaining sheets on the Basic Data form, as well as the Property Curves form, to enter optional information as described below.

Entering a Gravity Curve

If you do not enter a bulk gravity value on the Dist Curve sheet, you must enter a gravity curve using the Gravity/UOPK sheet. You may enter either:

- Gravity curve data
- Watson UOP K curve data

Gravities you specify on this sheet are normalized to match the bulk gravity value specified on the Dist Curve sheet.

To enter a gravity curve:

1. On the Gravity/UOPK sheet of the Components Assay/Blend Basic Data form, select the type of gravity data you wish to enter by clicking one of the options in the Type frame.
2. Enter at least four pairs of mid-percent and gravity values to define the profile in the columns for data.

If you enter a Watson UOPK curve, you must enter an average gravity on the Assay Basic Data Dist Curve sheet. If the distillation type is True Boiling Point (weight basis) or Vacuum (weight basis), you cannot enter a Watson UOPK curve.

Entering a Molecular Weight Curve

You can enter a molecular weight curve using the Molecular Wt sheet of the Assay/Blend Basic Input form. If you do not enter a molecular weight curve, Aspen Plus estimates it from the distillation curve and gravity you specify.

To enter a molecular weight curve:

➤ On the Molecular Wt sheet, enter at least four pairs of values in the Mid Percent Distilled and Molecular Weight fields to define the curve.

Entering Light-Ends Analysis

You can enter light-ends analysis for an assay in terms of the compositions of light-ends components. If you enter light-ends analysis, Aspen Plus does not generate pseudocomponents for the light-ends portion of the assay. If you wish to specify light-ends analysis, do this on the Light Ends sheet of the Components Assay/Blend Basic Data form.

To enter a light-ends analysis:

1. In the Light Ends Analysis frame of the Light Ends sheet, use the Component and Fraction columns to enter the component IDs and light ends fractions that make up the analysis. For your fractions, you can select a basis of Mass, Mole, or Standard Liquid Volume at the top of the column.
2. If the light-ends component is not in the databank, specify gravity and molecular weight in the Gravity and Molecular Weight fields of the analysis table.
3. Optionally, at the top of the sheet, enter the light-ends fraction as a fraction of the assay, in the Light Ends Fraction field.

   If you enter this value, the specified individual component fractions are normalized to this overall value. If you omit this value, individual component fractions are treated as fractions of the entire assay mixture.

Entering Petroleum Property Curves

You can enter any number of petroleum property curves for an assay, using the Petro Properties sheet of the Components Assay/Blend Property Curves form. Aspen Plus allows a variety of built-in curve types. Based on these curves, Aspen Plus assigns property values to individual pseudocomponents in the simulation.

Examples of petroleum properties include:

- Sulfur content
- Metal content
- Octane numbers

To enter petroleum property curves:

1. On the Petro Properties sheet, select a petroleum property in the Property Type list.
2. In the Property Curve Data frame, enter at least four pairs of values in the Mid Percent Distilled and Property Value fields, to define the curve.

3. Optionally, enter a bulk value for the property in the Bulk Value field. If you enter a bulk value, Aspen Plus normalizes the individual curve values to the bulk value.
4. To enter additional property curves, repeat steps 1 through 3 for each additional property.

Entering Viscosity Curves

You can enter viscosity curves at different temperatures for an assay using the Viscosity sheet of the Components Assay/Blend Property Curves form. Viscosity curves can be entered as either absolute or kinematic viscosity values as a function of percent distilled for the assay. Based on these curves, Aspen Plus will assign viscosity to pseudocomponents generated for the assay.

To enter viscosity curves:

1. On the Viscosity sheet of the Components Assay/Blend Property Curves form, choose a type of viscosity (Absolute or Kinematic) by clicking on the appropriate option in the Type frame.
2. In the Temperature list, select New.
3. In the New Item dialog box, enter a temperature for the viscosity curve, and click OK.
4. In the Mid Percent Distilled and Viscosity fields, enter at least four pairs of values to define the curve.
5. To enter viscosity curves at additional temperatures, repeat steps 1 through 5 for each curve.

To compute viscosity at multiple temperatures from the curves in the simulation, you must enter viscosity curves for at least two temperatures.

Creating a Blend

You can create a blend from any number of assays.

Aspen Plus performs blending on all available assay data:

- Distillation curves
- Gravity curves
- Molecular weight curves

- Light-ends analysis
- Petroleum properties curves
- Viscosity curves

Petroleum and viscosity curves are blended using the built-in or user-supplied blending rules. See Modifying Petroleum Property Definitions, this chapter.

When you define a stream using a blend, Aspen Plus automatically associates the petroleum properties and viscosity for the blend with the stream.

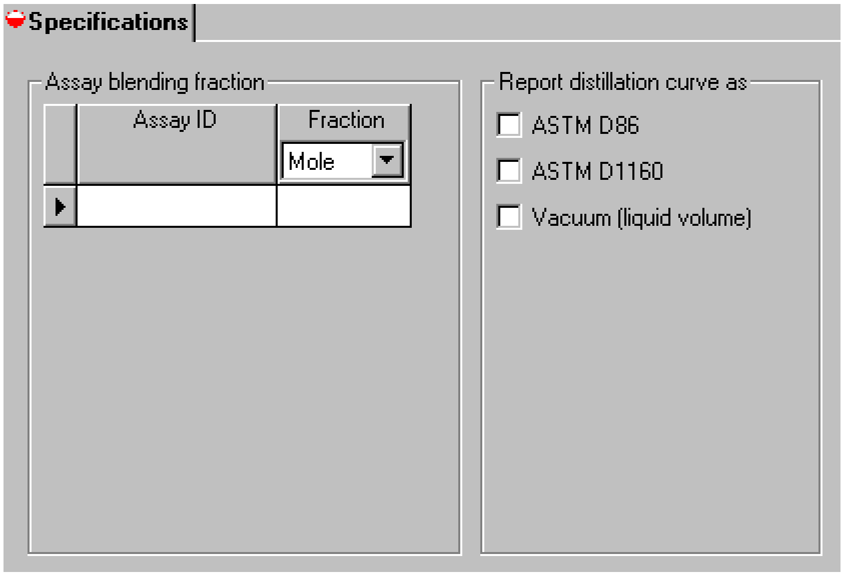
You can define a blend using either of the following:

- Components Specifications Selection sheet
- Assay-Blend Object Manager

Defining a Blend Using the Components Specifications Selection Sheet

To define a blend using the Components Specifications Selection sheet:

1. From the Data menu, select Components, then Specifications.
2. On the Components Specifications Selection sheet, enter a name for the blend in the Component ID field.
3. In the Type list, select Blend as the component type.
4. In the left pane of the Data Browser, click the Assay/Blend folder.
5. In the Assay/Blend Object Manager, select the Blend ID you just created, and click Edit. The Components Assay/Blend Mixture form appears:



To enter the blend specifications, see Entering Blend Specifications, this chapter.

Defining a Blend Using the Assay-Blend Object Manager

To define a blend using the Assay-Blend Object Manager:

1. From the Data menu, select Components, then Assay/Blend.
2. On the Assay-Blend Object Manager, click New.
3. In the Create New ID dialog box, choose Blend in the Select Type list.
4. Enter an ID for the blend, or accept the default ID.
5. Click OK.

   The Components Assay/Blend Mixture form appears. To enter the blend specifications, see Entering Blend Specifications, this chapter.

Entering Blend Specifications

To enter blend specifications, use the Specifications sheet of the Components Assay/Blend Mixture form:

1. On the Specifications sheet, select two or more assays in the Assay ID column, and specify the corresponding fraction of each assay, in the Fraction column. You can enter the assay blending fractions on a mole, mass or standard liquid volume basis.
2. By default Aspen Plus reports the distillation curve for the blend using the input basis and the true boiling point (liquid volume) basis. If you want to request additional distillation curve reports for the blend, you can specify this by clicking the desired curves in the Report Distillation Curve As frame.

Specifying Assay Analysis Options

Aspen Plus provides several options for:

- The assay data analysis procedure
- Converting and extrapolating distillation curves
- The initial and final boiling points for distillation curves

The defaults are appropriate for most applications.

To override the default options:

1. From the Data menu, select Components, then Petro Characterization.
2. In the left pane of the Data Browser window, click the Analysis Options folder.
3. On the Assay Procedures sheet, choose the preferred analysis procedure by clicking one of the options in the Assay Data Analysis Procedure frame:

   Version 9 or later

   \- or -

   Version 8 or earlier
4. In the Curve Processing Options frame, you can optionally modify any of the following specifications from their defaults:

Specification	Default
Initial boiling point	0.5
Final boiling point	99
Extrapolation method	Probability
Spline fitting method	Harwell

5. In the Distillation Curve Conversion Method frame, you can optionally modify the default conversion methods.

Modifying Petroleum Property Definitions

Aspen Plus has a list of pre-defined petroleum properties. You can enter property curves for these petroleum properties, as discussed in Entering Petroleum Property Curves, this chapter.

Examples of the built-in petroleum properties include:

- Sulfur content
- Metal content
- Freeze point

- Octane numbers

You can modify the definition of these pre-defined properties, or you can define new properties. See Defining a New Petroleum Property, this chapter.

To modify the definition of a petroleum property:

1. From the Data menu, select Components, then Petro Characterization.
2. In the left pane of the Data Browser window, click the Analysis Options folder.
3. On the Analysis Options form, select the Blend Options sheet.
4. In the Property list, select a petroleum property you wish to modify.
5. In the Blend Method field, select a property blending method.
6. If you are using a user blending subroutine, enter an option code in the Blend Option field. See *Aspen Plus User Models* for instructions on writing this subroutine.
7. If the property curve does not encompass 0 and 100 percent, specify whether it is to be extrapolated in the Extrapolate field.

About Pseudocomponents

You can specify how assays and blends are used to generate pseudocomponents. ADA/PCS can generate one or more sets of pseudocomponents for a group of assays and blends. You can use a particular assay or blend to generate only one set of pseudocomponents.

If you do not enter any specifications for pseudocomponent generation, ADA/PCS generates one average set of pseudocomponents for all the assays and blends. The average set uses equal weighting for each assay and blend.

You should use ADA/PCS to generate pseudocomponents only for assays and blends used to define flowsheet streams. This achieves the best characterization for a simulation. Typically you enter data for several assays to create a blend, then use the blend to define flowsheet streams. Generate pseudocomponents for the blend only.

In general, one average set of pseudocomponents for all assays and blends in the simulation is sufficient. Assign weighting factors to assays and blends to reflect their relative flow rates.

At times you can improve characterization accuracy by generating a separate set of pseudocomponents for each assay and blend. Use separate sets of pseudocomponents when multiple assays and blends define flowsheet streams, and in the assay/blend:

- Distillation curves have significant overlaps.
- Gravities and Watson K factors are very different.

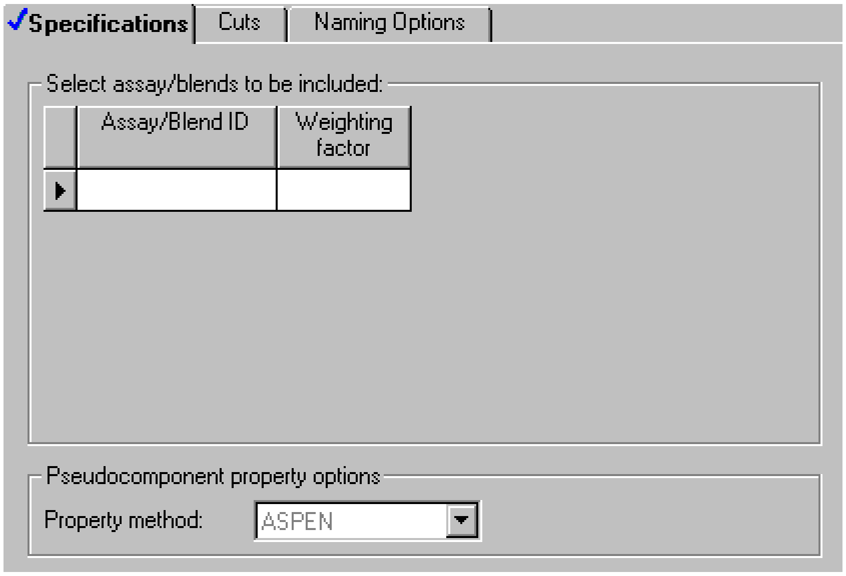
Multiple sets of pseudocomponents in the simulation increase computation time.

Entering Specifications for Generation of Pseudocomponents

To generate a set of pseudocomponents:

1. From the Data menu, select Components, then Petro Characterization.
2. In the left pane of the Data Browser window, select the Generation folder.
3. In the Generation Object Manager, click New.
4. In the Create New ID dialog box, enter an ID for the set of pseudocomponents, or accept the default ID.
5. Click OK.

   The Components Petro Characterization Generation form appears with the Specifications sheet selected:



Property method: ASPEN

6. On the Specifications sheet, select the assays and blends for which an average set of pseudocomponents is to be generated, using the Assay/Blend ID list.
7. In the Weighting Factor field, you can assign weighting factors to reflect the relative importance of each assay or blend in the generation of pseudocomponents. By default each assay or blend is given an equal weight of one.
8. At the bottom of the sheet, select a property method in the Property Method list. This property method represents the models to be used in the estimation of all pseudocomponent properties. By default ADA/PCS uses the ASPEN pseudocomponent property method to estimate pseudocomponent properties. See About Pseudocomponent Property Methods, this chapter, for a description of the built-in property methods.

Specifying Cut Points

By default Aspen Plus generates pseudocomponents using a standard set of cut points:

TBP Range (F)	Number of Cuts	Increments (F)
100 – 800	28	25
800 – 1200	8	50
1200 – 1600	4	100

To override the standard cut points, use the Cuts sheet on the Generation form to specify a list for one of the following:

- Cut temperatures
- Cut ranges. For each range, enter either the number of cuts or the temperature increment for each cut.

Pseudocomponent Naming Options

By default the generated pseudocomponents are named according to their mean average normal boiling point. You can use the Naming Options sheet on the Generation form to select from five built-in naming conventions. If you choose User Defined List, you must enter the pseudocomponent IDs in the Pseudocomponent fields of the Preview of Pseudocomponent Names frame. These IDs then appear on the Stream Input Specifications sheets, allowing you to enter pseudocomponent flows.

Defining Pseudocomponents and Entering Pseudocomponent Properties

In addition to allowing Aspen Plus to automatically generate pseudocomponents for your specified assays and blends, you also can choose to define pseudocomponents directly.

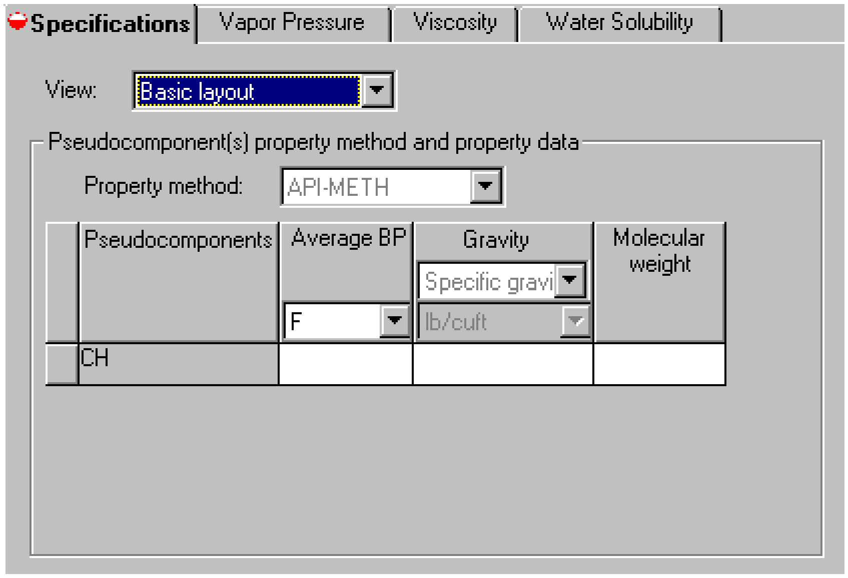
To create user-defined pseudocomponents, first enter them on the Components Specifications form:

1. From the Data menu, select Components, then Specifications.
2. On the Selection sheet, enter the names for the user-defined pseudocomponents in the Component ID fields.
3. Select PseudoComponent as the component type in the Type list. Leave the Component Name and Formula fields blank for pseudocomponents.

Entering Basic Properties for Pseudocomponents

Once the pseudocomponents are defined on the Components Specifications form, enter the basic properties for the pseudocomponent on the Components Pseudo Components Specifications sheet:

1. From the Data menu, select Components, then PseudoComponents.
   The Components PseudoComponents form appears with the Specifications sheet displayed:



View: Basic layout

Property method: API-METH

	Pseudocomponents	Average BP	Gravity	Molecular weight
			Specific gravi	
		F	lb/cuft	
	CH			

2. On the Specifications sheet, the pseudocomponents you defined on the Components Specification form are listed in the Pseudocomponents column. For each pseudocomponent, enter at least two of the following properties to characterize the pseudocomponent:

    - Average normal boiling point
    - Gravity/Density
    - Molecular weight

    Gravity or density can be entered in any of the following formats:

    - API gravity
    - Specific gravity
    - Standard liquid density

3. If you wish to modify the default pseudocomponent property method, select a new method in the Property Method list. About Pseudocomponent Property Methods, this chapter, for descriptions of the built-in option sets.

The default view of the PseudoComponents Specification sheet is the Basic Layout view. This view allows for a single pseudocomponent property method, and a single type of gravity or density to represent all pseudocomponents. If you wish to specify different property methods, or different types of gravity or density for individual pseudocomponents, you can select Advanced Layout from the View list at the top of the sheet. The Advanced Layout allows individual specifications of property methods and gravity or density types for each pseudocomponent.

Entering Temperature-Dependent Properties for Pseudocomponents

From the basic pseudocomponent properties you entered on the PseudoComponents Specifications sheet, Aspen Plus estimates all pure component properties needed for flowsheet simulation.

Optionally, you also can provide vapor pressure, viscosity, and water solubility data as a function of temperature for pseudocomponents. This improves the accuracy of the characterization.

To enter these temperature-dependent properties:

1. From the Data menu, select Components, then PseudoComponents.
2. On the Components PseudoComponents form, there are separate sheets for Vapor Pressure, Viscosity, and Water Solubility. Click the appropriate sheet for the type of data you wish to enter.
3. On the selected sheet, choose a pseudocomponent from the Component ID list.

4. In the frame below the Component ID, enter the property data as a function of temperature.
5. To enter data for other components, repeat steps 3 and 4.
6. To enter another property, repeat steps 2 through 4.

About Pseudocomponent Property Methods

A pseudocomponent property method is a collection of models for estimating pseudocomponent properties needed for flowsheet simulation. Pseudocomponent properties that are estimated include:

- Molecular weight
- Critical properties
- Acentric factor
- Vapor pressure
- Liquid molar volume
- Water solubility
- Viscosity
- Ideal gas heat capacity
- Enthalpy of vaporization
- Standard enthalpy and free energy of formation
- Equation of state properties

You can use a pseudocomponent property method in one of two ways:

On sheet	Specify a pseudocomponent property method for
Components Petro Characterization Generation Specifications	Pseudocomponents generated from assays
Components PseudoComponents Specifications	User-defined pseudocomponents

You can choose from five built-in pseudocomponent property methods:

Method	Description
API-METH	Uses procedures recommended by the American Petroleum Institute (API) Data Book.
COAL-LIQ	Uses correlations developed for coal liquids.
ASPEN	Based on the API-METH property method, with proprietary AspenTech enhancements for selected properties. (Default option set)
LK	Uses correlations by Lee and Kesler.
API-TWU	Based on the ASPEN property method, but uses correlations by Twu for critical properties.

You also can create your own pseudocomponent property methods. Use your own property methods in the same way as the built-in option sets. For details on creating your own pseudocomponent property methods, see the following section.

Creating Pseudocomponent Property Methods

You can create your own pseudocomponent property methods by starting with a built-in method, and modifying individual models for different pseudocomponent properties.

Aspen Plus provides several built-in models for each pseudocomponent property. Or you can supply your own model using a user-supplied subroutine. See *Aspen Plus User Models* for instructions on writing this subroutine.

To create a new pseudocomponent property method:

1. From the Data menu, select Components, then Petro Characterization.
2. In the left pane of the Data Browser window, click the Properties folder.
3. In the Petro Characterization Properties Object Manager, click New.
4. In the Create New ID dialog box, enter an ID (name) for the new method, or accept the default ID.
5. Click OK.
6. On the Basic sheet of the Properties form for the new method, select one of the built-in methods, by selecting from the Copy All Models From list. The chosen property method will be used as a basis for the new method.

   The remaining fields on the sheet (as well as the Thermodynamic sheet and the EOS sheet) display the models used by the base method for each property.

7. Use the remaining fields on the Basic sheet, the Thermodynamic sheet and the EOS sheet, to specify the property models which make up the property method.

Defining a New Petroleum Property

You can use a new petroleum property in the same ways as a pre-defined petroleum property. You can enter the curve data of this property for any assay. See Entering Petroleum Property Curves, this chapter.

You can define any number of additional petroleum properties to be used on the Prop-Sets Properties sheet and the Assay/Blend Property Curves form.

To define a new petroleum property:

1. From the Data menu, select Properties, then Advanced.
2. In the left pane of the Data Browser window, click the User Properties folder.
3. In the User Properties Object Manager, click New.
4. In the Create New ID dialog box, enter an ID (name) for the new property, or accept the default ID.
5. Click OK.
6. On the Specifications sheet of the Properties Advanced User Properties form, click the Assay Curve Property radio button at the top of the sheet.
7. In the Assay Curve Property Frame, select a blending method from the choices provided. The default method is Standard Liquid Volume Averaging.

   If you choose to use a user blending subroutine, enter an option code in the Blending Option field. See *Aspen Plus User Models* for instructions on writing this subroutine.
8. In the Default Property Used for Light Ends list, select a property to provide values for light-ends components.
9. At the bottom of the sheet, you can choose whether you want to extrapolate curve data that does not encompass the entire composition range (0-100%). Extrapolation is turned on by default. To turn off this option, click the check box to deselect it.
10. Click the Units sheet.
11. Click the appropriate check box to specify how you want the units conversion to be calculated.

12. If you choose to let Aspen Plus perform the units conversion, select the type of units in the Units type list.
13. If you choose to perform the units conversion in a user subroutine, enter a units label in the Units Label field. This label will be used in stream reports and property curve results.

Examining ADA/PCS Results

Aspen Plus produces a variety of ADA/PCS results. You can examine

- ADA results
- Pseudocomponent property results

Examining ADA Results

To examine ADA results:

1. From the Data menu, select Components, then Assay/Blend.
2. On the Assay/Blend Object Manager, select the assay or blend for which you want to display results, and click Edit.
3. In the left pane of the Data Browser window, click the Results form beneath the selected assay or blend.

   The Assay-Blend Results form appears, containing these sheets:

Sheet	Shows
Light Ends Analysis	Results of the light ends analysis
Pseudocomp Breakdown	Pseudocomponent and light ends breakdown results
Curves	Distillation curves and bulk properties results
Blend Fraction (Blends only)	Compositions of blends

4. From the Curves sheet, you can generate plots of distillation temperatures versus percent distilled. See chapter 13 for instructions on generating plots.

Examining Pseudocomponent Property Results

To examine pseudocomponent property results:

1. From the Data menu, select Components, then Petro Characterization.
2. In the left pane of the Data Browser, click the Results folder.

   The Summary sheet on the Components Petro Characterization Results form displays the key properties for each pseudocomponent in table format.
3. You can generate plots of pseudocomponent properties versus boiling points or any other property. See Chapter 13 for instructions on generating plots.

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