# COMThermo Workbench™ 2.2

## *Thermodynamic Workbench Guide*

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# Table of Contents

# 1 Thermodynamic Workbench Manager

# 1.1 Introduction

The Thermodynamic Workbench Manager view is used to access, create, or delete the following operations:

- Phase Equilibrium
- Property Table
- Pure Component Regression
- Fluid Phase Regression

These operations are thermodynamic tools that allow you to explore thermodynamic model behaviour and properly determine and tune interaction parameters and physical properties.

## 1.1.1 Phase Equilibrium

The Phase Equilibrium operation allows you to assess the quality of the thermodynamic model that has been selected to represent a mixture. The operation enables the visualization of key properties for binary and ternary mixtures.

### General Procedure

To generate a Phase Equilibrium Properties operation:

1. Create a fluid package containing the necessary components and property package.
2. From the **Features** menu, select **Phase Equilibrium**. The Phase Equilibrium view appears.
3. Click the **Setup** tab.
4. Select the components you want to analyze.
5. Click the **Plots** tab.
6. Set the plot parameters options. The plot appears in the view.

The Plots tab appears only after you have selected components on the Setup tab.

# 1.1.2 Property Table

The Property Table allows you to examine what happens to components and component streams when you apply different property values.

## General Procedure

To create a Property Table:

1. Create a fluid package containing the necessary components and property package.
2. From the **Features** menu, select **Property Table**. The Property Table view appears.
3. Click the **Setup**.
4. Select the appropriate fluid package, fraction basis, independent variable(s), and properties to be calculated.
5. Click the **Table** tab.
6. Enter feed conditions. Property Table operation automatically calculates the remaining properties.
7. Click the **Plots** tab.
8. Select the dependent variable and phase setting to create property curves.

# 1.1.3 Fluid Phase Regression

When designing or evaluating any process, the representation of the phase equilibrium is fundamental to the accuracy of the simulation. The Fluid Phase Regression operation allows you to derive interaction coefficients that are optimized for the process being considered.

## General Procedure

To create a Fluid Phase Regression:

1. Create a fluid package containing the necessary components and an appropriate property package.
2. From the **Features** menu, select **Fluid Phase Regression**. The Fluid Phase Regression view appears.
3. Click the **Summary** tab.
4. Select a data set or create a data set to calculate the new binary interaction parameter values.
5. Click the **Variables** tab.
6. Examine the default values of the binary interaction parameter values and select the degrees of freedom status for the binary interaction parameters.
7. To verify if the data set is appropriate, examine the information on the **Consistency**, **Error**, and **Error Plots** tabs.
8. Click the **Optimizer** tab, then click the **Optimize** button. You will see the progress of the optimization calculation.
9. Click to the **Variables** tab to view the new values for the binary interaction parameter values based on the selected data set.

# 1.1.4 Pure Component Regression

The Pure Component Regression operation allows you to create new components or modify existing ones for specific process considerations.

Coefficients for more than twenty-five thermophysical properties can be regressed using a wide range of equation forms. Multiple data sets can be employed, using different weighting factors for each set or individual points within the set. This allows you to quickly compare the fit of the calculated data vs. the experimental data.

## General Procedure

To create a Pure Component Regression:

1. Create a fluid package containing the necessary components and an appropriate property package.
2. From the **Features** menu, select **Pure Component Regression**. The Pure Component Regression view appears.
3. Click the **Data** tab.
4. On the **Data** tab, create a new data set and enter the experimental information.
5. Click the **Plots** tab to compare the experimental data graphically with the regression module's data.
6. Click the **Errors** tab, then click the **Regress** button to regress the new values for the equation.

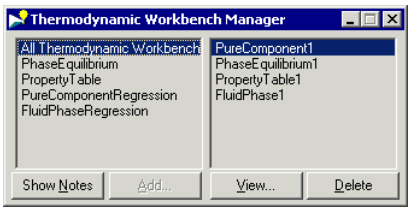
# 1.2 Thermodynamic Workbench Manager View

To access the Thermodynamic Workbench Manager view, do one of the following:

Thermodynamic Workbench Manager icon

- Click on the **Thermodynamic Workbench Manager** icon in the tool bar.
- From the **Managers** menu, select **Thermodynamic Workbench Manager**.

**Figure 1.1**




The Thermodynamic Workbench Manager view contains four buttons used to manipulate the thermodynamic operations:

| Button | Description |
|---|---|
| **Show/Hide Notes** | Allows you to access the notes associated with the operations. |
| **Add** | Allows you to add a thermodynamic operation. |
| **View** | Allows you to access existing operations for the case. |
| **Delete** | Allows you to delete existing operations from the case. |

## 1.2.1 Adding an Operation

To add an operation:

Thermodynamic Workbench Manager icon

1. Open the Thermodynamic Workbench Manager view.
2. In the list on the left, select the type of operation you want to add.
3. Click the **Add** button. The property view for the selected operation appears.

## 1.2.2 Editing an Operation

To edit an existing operation:

1. Open the Thermodynamic Workbench Manager view.
2. In the list on the left, select the type of operation you want to edit. To see all existing operations available, select **All Thermodynamic Workbench** from the left list.
3. From the list on the right, select the operation you want to edit.
4. Click the **View** button. The property view for the selected operation appears.

## 1.2.3 Deleting an Operation

To delete an existing operation:

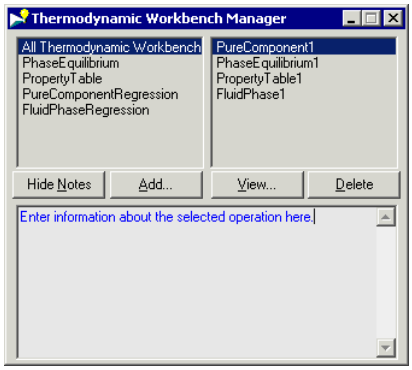
1. Open the Thermodynamic Workbench Manager view.
2. In the list on the left, select the type of operation you want to edit. To see all existing operation available, select **All Thermodynamic Workbench** from the left list.
3. From the list on the right, select the operation you want to delete.
4. Click the **Delete** button.
5. Thermodynamic Workbench Manager will prompt you to confirm that you want to delete the selected operation.
   Click the **Yes** button to delete the selected operation, or click the **No** button to keep the selected operation.

# 1.2.4 Editing Operation Notes

To edit the notes associated with the operation:

1. Open the Thermodynamic Workbench Manager view.
2. In the list on the left, select the type of operation you want.
   To see all existing operations available, select **All Thermodynamic Workbench** from the left list.
3. From the list on the right, select the operation to which you want to add notes.
4. Click the **Show Notes** button. A text editor appears at the bottom of the Thermodynamic Workbench Manager view.

**Figure 1.2**




5. Edit the notes associated with the selected operation.
   If there have been no previous notes entered for the selected operation, the text editor will appear blank.

**The notes text editor associated with the selected operation is connected to the Notes tab of the selected operation. Any changes made to the information in this notes text editor will also appear in the Notes tab of the operation, and vice versa.**

6. Once you have completed editing the notes, click the **Hide Notes** button to collapse the notes text editor.

# 2 Phase Equilibrium

# 2.1 Introduction

The Phase Equilibrium operation is used to assess the quality of the thermodynamic model that has been selected to represent a mixture. The operation enables the visualization of key properties for binary and ternary mixtures.

With the Phase Equilibrium operation, the degree of precision required when modeling your process has never been greater. The foundation of any modeling is the accurate representation of the pure component behaviour and vapour-liquid or liquid-liquid equilibrium. For non-ideal mixtures in particular, the behaviour of a system can vary greatly depending on the process conditions. Optimizing your component libraries for your specific situation will ensure the most accurate model possible.

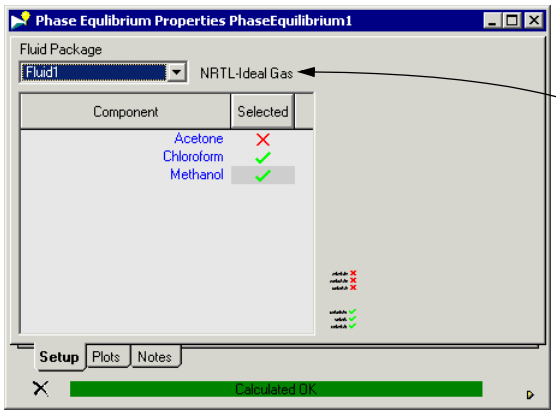
# 2.2 Phase Equilibrium View

To access a Phase Equilibrium operation, do one of the following:

- From the **Features** menu, select **Phase Equilibrium Properties**.
- From the **Managers** menu, select **Thermodynamic Workbench Manager**. The manager view appears. In the left list, select **PhaseEquilibrium**, then click the **Add** button.

To access previously created Phase Equilibrium operations, refer to **Section 1.2.2 - Editing an Operation**.

**Figure 2.1**




The Phase Equilibrium view contains three objects and two or three tabs at the bottom of the view. The following table describes each object:

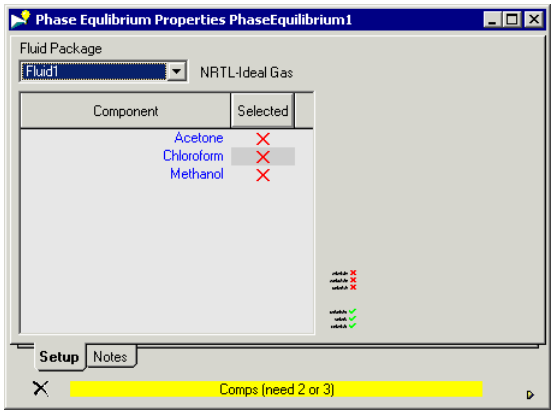
| Object | Icon | Description |
|---|---|---|
| **Delete icon** | | Allows you to delete the current Phase Equilibrium operation. |
| **Status bar** | | Displays the status of the current Phase Equilibrium operation. |
| **Opens Current Page in Separate Window icon** | | Allows you to open the active tab as a separate view. |

The status bar at the bottom of the view indicates the status of the operation or the information required before the operation can generate results.

# 2.2.1 Setup Tab

The Setup tab allows you to select the fluid package and components you want to analyze.

**Figure 2.2**




The following table lists and describes the objects available in the Setup tab:

| Object | Icon | Description |
|---|---|---|
| **Fluid Package drop-down list** | | Allows you to select the fluid package you want to analyze. |
| **Component column** | | Displays all the components in the selected fluid package. |
| **Selected column** |   | Allows you to toggle the selection status of the components by clicking the on icon in the column.<br>• A green checkmark indicates that the component is selected.<br>• A red cross indicates that the component is not selected. |
| **Unselect All Components icon** |  | Allows you to deselect all the components in the fluid package. |
| **Select All Components icon** |  | Allows you to select all the components in the fluid package. |

You can select up to three components. After you select two or three components, the Plots tab appears.

# 2.2.2 Plots Tab

The Plots tab is available only if you have selected two or three components in the Setup tab.

The Plots tab allows you to assess the quality of the thermodynamic model/property package for the selected group of components in a plot format.

The Plots tab displays either a Binary plot or a Ternary plot. The type of plot that appears in the Plots tab depends on how many components you selected in the Setup tab.

The following sections describes each plot type.

## Binary Plot

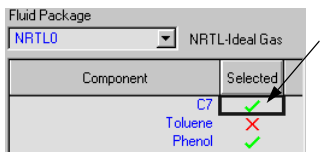
To access a binary plot:

1. Open the Phase Equilibrium view.
2. Click the **Setup** tab.
3. In the **Setup** tab, use the Fluid Package drop-down list to select a fluid package with two or more components.
4. In the **Selected** column, click the icons to select two components from the fluid package.
   After selecting two components, the **Plots** tab appears between the **Setup** tab and **Notes** tab.

A green checkmark ✓ indicates that the component is selected.

A red cross ✗ indicates that the component is not selected.

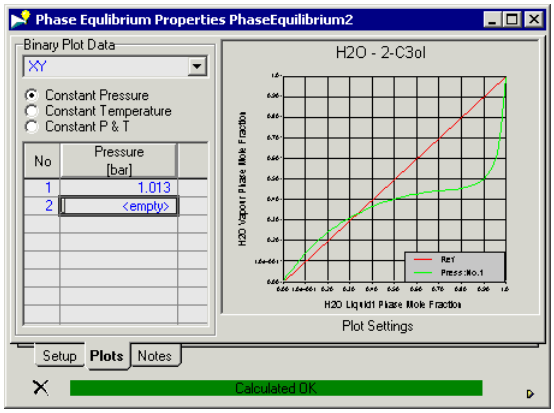
**Figure 2.3**




Click the green checkmark to unselect a component, or click a red cross to select a component.

5. Click the **Plots** tab.

**Figure 2.4**




The following table lists and describes the objects/options available in the Plots tab for a binary plot:

| Object | Description |
|---|---|
| **Binary Plot Data drop-down list** | Allows you to select the binary plot type that will appear in the plot.<br>There are fifteen types of plot to choose from:<br>• XY<br>• TXY — Available only for the Constant Pressure option.<br>• PXY — Available only for the Constant Temperature option.<br>• K-Value<br>• Relative Volatility<br>• Activity Coefficient<br>• Fugacity Coefficient<br>• Gibbs Excess-X<br>• Gibbs Mixture-Available only for the Constant P&T option.<br>• Enthalpy<br>• Entropy<br>• Molar Density<br>• Viscosity<br>• Thermal Conductivity<br>• Surface Tension |
| **Constant Pressure radio button** | Allows you to limit the calculations of the plot to specific constant pressures. |
| **Constant Temperature radio button** | Allows you to limit the calculations of the plot to specific constant temperatures. |

| Object | Description |
|---|---|
| **Constant P & T** | Allows you to limit the calculations of the plot to specific constant pressures and constant temperatures. |
| **Binary Plot Data table** | Allows you to enter up to five independent pressures and/or temperatures (depending on your selection of the above radio buttons) for the creation of the binary plots. |
| **Plot** | Displays the binary plot depending on the options entered in the Binary Plot Data group.<br>The plot will appear blank until you enter pressures and/or temperatures into the Binary Plot Data table. |
| **Plot Settings button** | Allows you to access the Plot Settings view. This view allows you to manipulate the plot. See the **Plot Settings View** section for more information. |

Refer to **Chapter 8 - Plot Properties** and **Section 7.4 - Plot Area** in the **User Guide** for more information about how to customize or print the plot.

## Plot Settings View

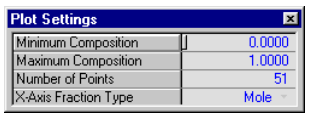
The Plot Settings view allows you to manipulate the following:

- The range of composition fractions displayed in the plot.
- The number of calculated points displayed in the plot.
- The composition fraction type displayed in the plot.

To access the Plot Settings view:

1. Open the Phase Equilibrium view.
2. Click the **Setup** tab.
3. In the **Setup** tab, select a fluid package, then select two components from the fluid package.
4. Click the **Plots** tab, then click the **Plot Settings** button.

**Figure 2.5**




The following table lists and describes the options available on the Plot Settings view:

| Binary Plot Setting | Description |
|---|---|
| **Minimum Composition cell** | Allows you to set the minimum composition fraction for the plot. |
| **Maximum Composition cell** | Allows you to set the maximum composition fraction for the plot. |

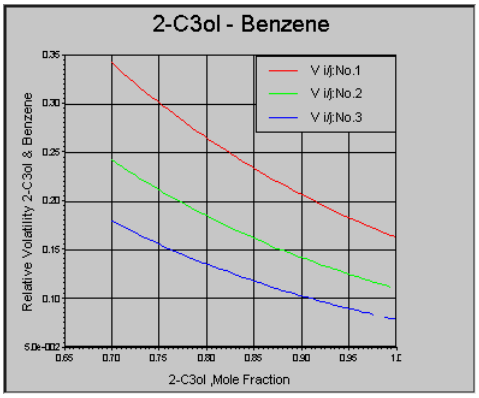
The Minimum and Maximum Composition settings are useful when you want to examine a certain region in detail. This can be useful for determining whether or not an azeotrope exists.

| Binary Plot Setting | Description |
|---|---|
| **Number of Points cell** | Allows you to set the number of calculated points in each curve. The default value is 51 and is acceptable for most cases. |
| **X-Axis Fraction Type drop-down list** | Allows you to set the composition basis for the x-axis as Mass Fraction, Mole Fraction, or Standard Liquid Volume Fraction. |

The Standard Liquid Volume Fraction option should be used with caution. Although this option is unconditionally provided, it does not make sense to use it for "vapour-like" components such as Hydrogen.

The figure below shows a focused plot view of the Relative Volatility for Benzene-2-C3ol using the Plot Settings options.

**Figure 2.6**




# Ternary Plot View

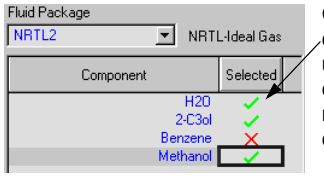
To access a ternary plot:

1. Open the Phase Equilibrium view.
2. Click the **Setup** tab.
3. In the **Setup** tab, use the **Fluid Package** drop-down list to select a fluid package with three or more components.
4. Click the icons in the **Selected** column to select three components from the fluid package.

A green checkmark indicates that the component is selected.

A red cross indicates that the component is not selected.

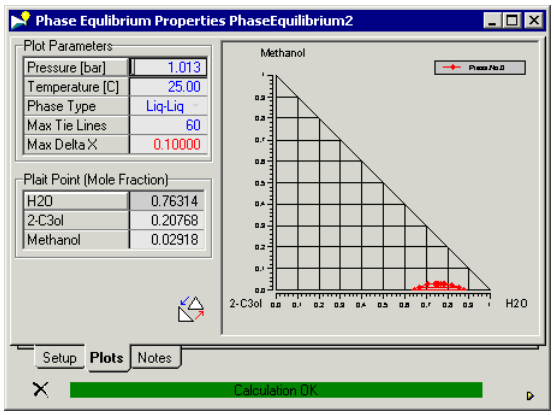
**Figure 2.7**




Click the green checkmark to unselect a component, or click a red cross to select a component.

5. Click the **Plots** tab.
6. In the **Pressure** and **Temperature** cells, enter appropriate values.
7. in the **Phase Type** cell, select a phase type from the drop-down list.

**Figure 2.8**




Vapour-Liquid regions will not be detected if you have selected Liquid-Liquid for the Phase Type, and vice versa.

Unlike the binary plot, the ternary plot has only two types of plots: Liquid-Liquid phase or Vapour-Liquid phase. The ternary plot is also strictly for two-phase equilibrium (LLE or VLE). Three-phase equilibrium (VLLE) is not supported in this plot.

The following table lists and describes the objects available in the Plots tab for a ternary plot:

| Object | Icon | Description |
|---|---|---|
| **Pressure cell** | | Allows you to specify the pressure for the ternary plot. |
| **Temperature cell** | | Allows you to specify the temperature for the ternary plot. |
| **Phase Type drop-down list** | | Allows you to select between Liq-Liq phase or Vap-Liq phase plots.<br>If you select Liq-Liq, any liquid-liquid regions at the selected pressure and temperature will appear on the ternary plot.<br>If you select Vap-Liq, any vapour-liquid regions at the selected pressure and temperature will appear on the ternary plot.<br>Azeotropes are not calculated here; they are calculated in Residue Curve Map operation. Refer to **Chapter 6 - Residue Curve Map** in the **Azeotropic Separation** manual for more information. |

The liquid-liquid regions are found by checking points along the boundaries of the composition triangle. If your system has a two-phase region which is entirely within the composition triangle (not touching any edges), it will not be detected when plotting the Liquid-Liquid regions.

| Object | Icon | Description |
|---|---|---|
| **Max Tie Lines cell** | | Allows you to set the maximum number of ties lines displayed in a liquid-liquid or vapour-liquid region. |
| **Max Delta X cell** | | Allows you to set the maximum step taken in the calculation of the tie lines.<br>In addition to controlling the appearance of the envelope, the Max Delta X setting can also be useful in stabilizing the calculations. The calculation scheme uses the previous tie line to initialize the calculation of the next one. Decreasing the maximum change allowed constantly provides better initial guesses for the next calculation step. If the phase envelope looks unlikely, try lowering the maximum change allowed and rerunning the problem. |
| **Plait Point table** | | Displays the mixture's composition when the liquid-liquid envelope first appears at a point on the graph. |
| **Select Triangle Type icon** |  | Allows you to toggle between displaying the plot as a right angle triangle or as an equilateral triangle. |

If the MaxDeltaX setting is decreased, it is advisable to increase the maximum number of tie lines allowed.

# 2.2.3 Notes Tab

The Notes tab allows you to:

- Change the name of the Phase Equilibrium operation by entering a new name in the **Name** field.
- Enter information regarding the Phase Equilibrium operation in the **Notes** text editor.

Any changes made to the information in the Notes text editor will appear in the text editor located at the bottom of the Thermodynamic Workbench Manager view when the Show Notes button has been clicked.

# 3 Property Table

# 3.1 Introduction

The Property Table operation allows you to examine the chemical properties of a set of components at various operating conditions in a graphical or tabular format. Properties can be calculated for streams created in the Stream Manager or individual components based on specified feed conditions such as Temperature, Pressure, Enthalpy, Vapour Fraction, Composition, or Stream flow rate.

In general, any two of the properties mentioned above must be specified with a third property set to vary over a given range. The Property Table operation then calculates the remaining properties over the selected range.

## 3.1.1 Independent Variables

One or two variables can be set to vary in a Property Table operation. If two independent variables are selected, a three dimensional Property Table will be generated. The default number of independent variables for a Property Table is 1. If two independent variables are specified then another set of fields appears at the bottom of the screen.

### Specification of Independent Variables

The independent variables, their boundary conditions, and the number of points to calculate are specified in a set of fields at the bottom of the Setup tab of the Property Table view. These conditions may vary depending on the composition basis you select.

If you select a Component Basis, then the composition of any component present in the active fluid package can be specified as an independent variable. Alternatively, the phase fraction, pressure, temperature, or enthalpy can also be specified.

For more information about the stream, refer to **Chapter 6 - Stream Manager**.

If a Stream Basis has been selected, then any stream can be specified as an independent variable. The Property Table operation is designed to use only streams with complete component composition specifications. When a stream basis is used, the boundary conditions represent flow

rates. Alternatively, the phase fraction, pressure, temperature, or enthalpy can also be specified.

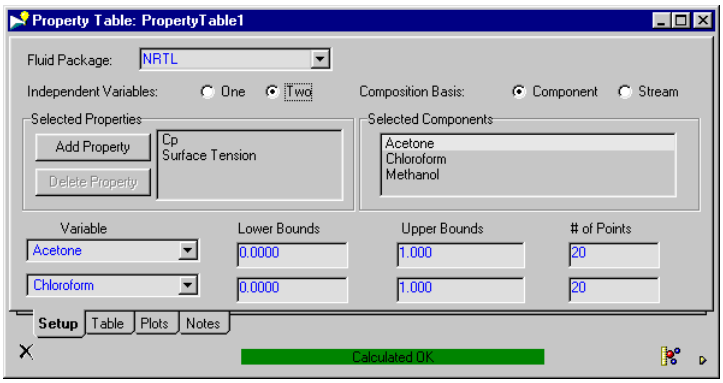
# 3.2 Property Table View

To access the Property Table view, do one of the following:

- From the **Features** menu, select **Property Table**.
- From the **Managers** menu, select **Thermodynamic Workbench Manager**. The manager view appears. From the left list, select **PropertyTable**, then click the **Add** button.

To access previously created Property Table operations, refer to **Section 1.2.2 - Editing an Operation**.

**Figure 3.1**




The Property Table view contains four tabs: Setup, Table, Plots, and Notes. The view also contains four objects. The following table lists and describes the four objects located at the bottom of the view:

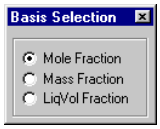
| Object | Icon | Description |
|---|---|---|
| **Delete icon** | | Allows you to delete the current Property Table operation. |
| **Status bar** | | Displays the status of the current Property Table operation. |
| **Change... Basis icon** | | Allows you to change the composition fraction basis displayed in the current Property Table view. |
| **Open... Window icon** | | Allows you to open the active tab as a separate view. |

For more information about the composition fraction basis, refer to the **Basis Selection View** section.

# Basis Selection View

The Basis Selection view allows you to change the composition basis fraction type displayed in the Property Table view.

**Figure 3.2**




Change Composition Fraction Basis icon

To change the composition basis using the Basis Selection view:

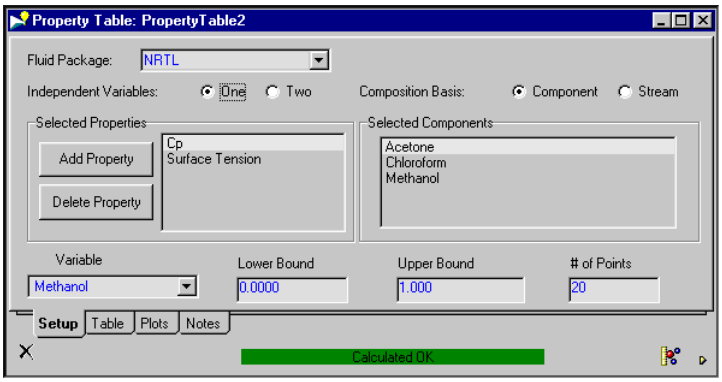
1. Click the **Change Composition Fraction Basis** icon to open the Basis Selection view.
2. Use the radio buttons to select the composition basis you want to display in the Property Table view.
3. Click the **Close** icon when you are done.

The following sections describe in detail each tab available in the Property Table view.

# 3.2.1 Setup Tab

The Setup tab allows you to select the fluid package, independent variable, and dependant variable for analysis.

**Figure 3.3**




The following table lists and describes the objects available in the Setup tab:

| Object | Description |
|---|---|
| **Fluid Package drop-down list** | Allows you to select the fluid package that contains the components and property package you want to analyze. |
| **Independent Variables radio buttons** | Allows you to select one or two independent variables for the property analysis. |
| **Composition Basis radio buttons** | Allows you to select the components in the fluid package or streams from the Stream Manager for analysis.<br>Select the Component radio button to analyze the components in the fluid package.<br>Select the Stream radio button to analyse the streams from the Stream Manager. For more information about streams, refer to **Chapter 6 - Stream Manager**. |
| **Selected Properties list** | Displays the dependent variables/properties you have selected for analysis. |
| **Add Property button** | Allows you to access the Property Selector view, which allows you to add dependent variables/properties to the Property Table operation. Refer to the **Adding Dependant Variables** section for more information. |
| **Delete Property button** | Allows you to remove dependant variables/properties from the Property Table operation. Refer to the **Removing Dependant Variables** section for more information. |

The Property Table operation is designed to use only streams with complete component composition specifications.

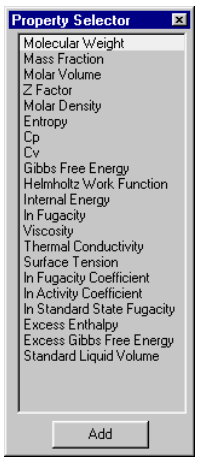
| Object | Description |
|---|---|
| **Selected Components list** | Displays all the components in the fluid package available for analysis. This group is available only if the Component radio button is selected. |
| **Selected Streams list** | Displays all the streams selected for analysis. This group is available only if the Stream radio button is selected. |
| **Add Stream button** | Allows you to access the Available Streams view, which allows you to add streams to the Property Table operation. Refer to the **Adding Streams** section for more information. |
| **Remove Stream button** | Allows you to remove selected streams from the Property Table operation. Refer to the **Removing Streams** section for more information. |
| **Variable drop-down list** | Allows you to select an independent variable for analysis. |
| **Lower Bounds field** | Allows you to specify the lowest value for the associated independent variable. |
| **Upper Bounds field** | Allows you to specify the highest value for the associated independent variable. |
| **# of Points field** | Allows you to specify how many data points you want calculated and plotted. |

If the Two radio button was selected for the independent variable, there will be two of the following: Variable drop-down lists, Lower Bounds fields, Upper Bounds fields, and # of Points fields.

# Adding Dependant Variables

To add dependant variables/properties to the Property Table operation:

1. Open the Property Table view.
2. Click the **Setup** tab.
3. In the **Fluid Package** drop-down list, select the fluid package that contains the components and property package you want to analyze.
4. In the Selected Properties group, click the **Add Property** button. The Property Selector view appears.
5. Select the dependant variable/property from the list of properties in the view, then click the **Add** button.
6. Repeat step #5 until you have added all the properties you want to add.
7. Click the **Close** icon to close the Property Selector view.




Property Selector view

# Removing Dependant Variables

To remove dependant variables/properties from the Property Table operation:

1. Open the Property Table view.
2. Click the **Setup** tab.
3. In the Selected Properties list, select the dependant variable you want to remove.
4. Click the **Delete Property** button.
5. Repeat steps #3 and #4 until you have removed all the unneeded dependant variables.

You can also press the DELETE key to remove the selected property.

# Adding Streams

To select a stream from the Stream Manager:

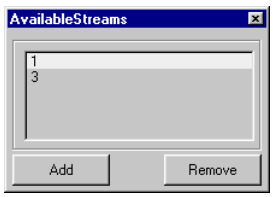
1. Open the Property Table view.
2. Click the **Setup** tab.
3. In the Fluid Package drop-down list, select the fluid package that contains the streams you want to analyze.
4. In the Selected Streams group, click the **Add Stream** button. The Available Streams view appears.

The Property Table operation is designed to use only streams with complete component composition specifications.

The Available Streams view allows you to both add and remove streams from the Property Table operation.

To remove a stream, select the stream's name on the Available Streams view and click the **Remove** button.

**Figure 3.4**




5. From the list, select the stream you want to add, then click the **Add** button.
6. After selecting all the streams required, click the **Close** icon to close the Available Streams view.

# Removing Streams

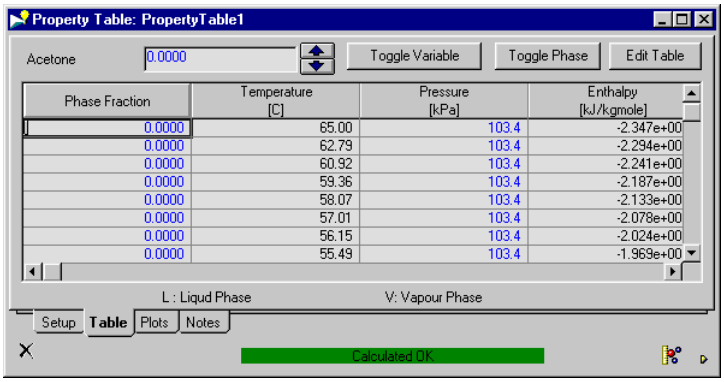
To remove streams from the Property Table operation:

1. Open the Property Table view.
2. Click the **Setup** tab.
3. In the Selected Streams list, select the stream you want to remove.
4. Click the **Remove Stream** button.
5. Repeat steps #3 and #4 until you have removed all the unneeded streams.

# 3.2.2 Table Tab

The Table tab displays the calculated variables in table format.

**Figure 3.5**




The following table lists and describes the objects available in the Table tab. The objects available in the Table tab vary depending on whether you selected one or two independent variables.:

| Object | Description |
|---|---|
| ***Independent* variable field** | Allows you to modify the independent variable value by clicking the Spinner icon to increase or decrease the value. Available only if Two independent variables are selected in the Setup tab. |
| **Name field** | Allows you to edit the name of the current Property Table operation. Available only if One independent variable is selected is selected in the Setup tab. |

Spinner icon

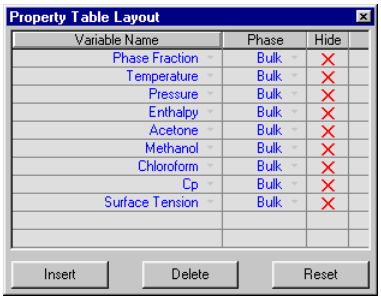
| Object | Description |
|---|---|
| **Toggle Variable button** | Allows you to toggle between the first and second independent variable that will be specified in the Independent variable field. Available only if Two independent variables are selected in the Setup tab. |
| **Toggle Phase button** | Allows you to toggle the calculated results for a liquid phase or vapour phase. In liquid phase, the column names are accompanied by *(L)*. In vapour phase, the column names are accompanied by *(V)*. |
| **Edit Table button** | Allows you to access the Property Table Layout view. This view allows you to manipulate the information displayed on the table. Refer to the **Property Table Layout View** section for more information. |
| **Table** | Displays the calculated values of the dependant variables and the specified values from the independent variables and components/ streams.<br>You need to specify at least one dependant variable in the table before calculation analysis begins. |

Depending on your selection in the Setup tab, you may need to specify multiple dependant variables in the table.

# Property Table Layout View

The Property Table Layout view allows you to manipulate the information displayed in the Table tab.

**Figure 3.6**




The following table lists and describes the objects available in the Property Table Layout view:

| Object | Description |
|---|---|
| **Variable Name column** | Displays the all properties/variables selected for the Property Table operation. |
| **Phase column** | Displays the type of phase associated with the variable that will appear in the Table tab.<br>Use the drop-down list option in the Phase cells to select a different phase type. There are three phase types available: Bulk, Liquid, and Vapour. |
| **Hide column** | Indicates whether the associated variable is hidden or displayed in the Table tab. |
| **Insert button** | Allows you to insert a variable row. |
| **Delete button** | Allows you to remove a selected variable from the Table tab. |
| **Reset button** | Allows you to reset the information on the Table tab back to the program's default settings. |

A red cross indicates that the variable appears on the Table tab.

A green checkmark indicates that the variable is hidden.

There are three ways to manipulate the variables/information displayed on the Table tab:

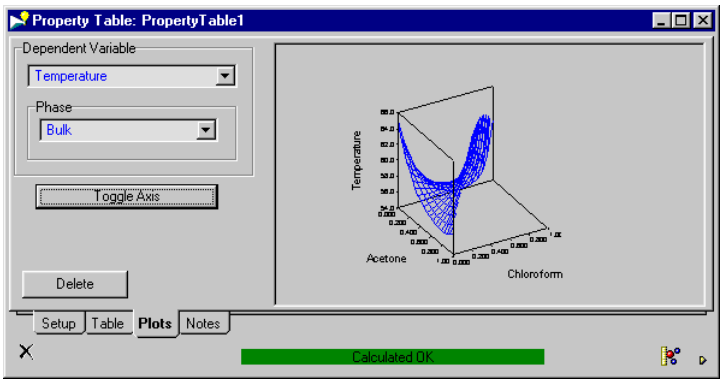
- Use the drop-down list options in the Variable Name cells to select different variables.
- Check or uncheck the Hide cells to hide or display the variables.
- Use the **Insert** and **Delete** buttons to add or remove the variables.

# 3.2.3 Plots Tab

The objects on the Plots tab varies depending on whether you selected one or two independent variables in the Setup tab.

The Plots tab allows you to view the calculated results of the variables/ properties in a plot format.

**Figure 3.7**




The following table lists and describes the objects available in the Plots tab:

For the binary plot, you can select multiple dependant variables.

| Object | Description |
|---|---|
| **Dependent Variable drop-down list** | Allows you to select the dependant variable that will appear on the plot. |
| **Phase drop-down list** | Allows you to select the type of phase used to calculate the dependant variable values that will appear on the plot. |
| **Toggle Axis button** | Allows you to flip the axis position of the two independent variables. Available only if two independent variables were selected on the Setup tab. |
| **Delete button** | Allows you to remove the selected dependant variable from the plot. Available only for binary plots. |
| **Clear All button** | Allows you to remove all dependant variables from the plot. Available only for binary plots. |
| **Plot** | Displays the selected dependant and independent variable values in a plot format.<br>For one independent variable, the plot is a binary plot.<br>For two independent variables, the plot is a quaternary plot. |

For information about manipulating plot appearance, refer to **Section 7.4 - Plot Area** and **Chapter 8 - Plot Properties** in the **User Guide**.

# 3.2.4 Notes Tab

The Notes tab allows you to:

- Change the name of the Property Table operation by entering a new name in the **Name** field.
- Enter information regarding the Property Table operation the **Notes** text editor.

Any changes made to the information in the Notes text editor will appear in the text editor located at the bottom of the Thermodynamic Workbench Manager view when the Show Notes button has been clicked.

# 4 Pure Component Regression

# 4.1 Introduction

The Pure Component Regression operation allows you to enter your own temperature dependent property data from which coefficients can be regressed for the appropriate equation. You can choose from a number of temperature dependent properties listed below:

| Temperature Dependent Properties | |
|---|---|
| Solid Density | Gas Liquid Surface Tension |
| Liquid Density | PRMathias Copeman |
| Vapour Pressure | Ideal Gas Gibbs Free Energy |
| Sublimation Pressure | Gas Density |
| Enthalpy of Vapourization | Solid Thermal Conductivity |
| Solid Heat Capacity | K Value1 |
| Liquid Heat Capacity | K Value2 |
| Ideal Gas Enthalpy | Separation Factor |
| Second Virial Coefficient | Solid Enthalpy |
| Liquid Viscosity | Liquid Enthalpy |
| Gas Viscosity | Gas Enthalpy |
| Liquid Thermal Conductivity | Solid Entropy |
| Gas Thermal Conductivity | Liquid Entropy |
| Gas Heat Capacity | Gas Entropy |

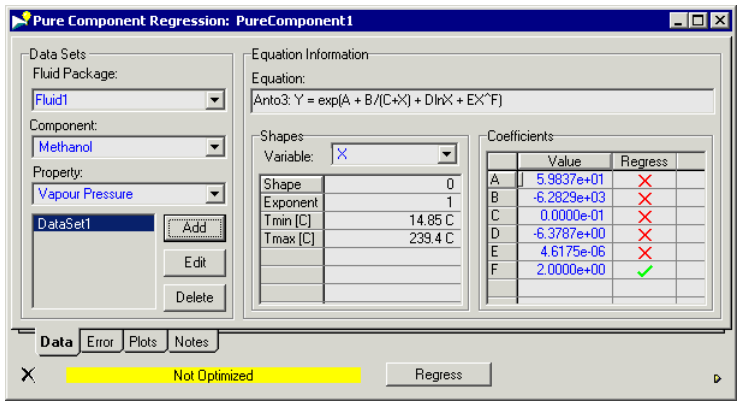
# 4.2 Pure Component Regression View

To access the Pure Component Regression view, do one of the following:

- From the **Features** menu, select **Pure Component Regression**.
- From the **Managers** menu, select **Thermodynamic Workbench Manager**. The manager view appears. In the left list, select **PureComponentRegression**, then click the **Add** button.

To access previously created Property Table operations, refer to **Section 1.2.2 - Editing an Operation**.

**Figure 4.1**




The Pure Component Regression view contains four tabs: Data, Error, Plots, and Notes. The view also contains four objects. The following table lists and describes the four objects located at the bottom of the view:

| Object | Icon | Description |
|---|---|---|
| **Delete icon** | | Allows you to delete the current Pure Component Regression operation. |
| **Status bar** | | Displays the status of the current Pure Component Regression operation. |
| **Regress button** | | Allows you to regress the equation's coefficient values to match the data from the entered data set. |
| **Opens Current Page in Separate Window icon** | | Allows you to open the active tab as a separate view. |

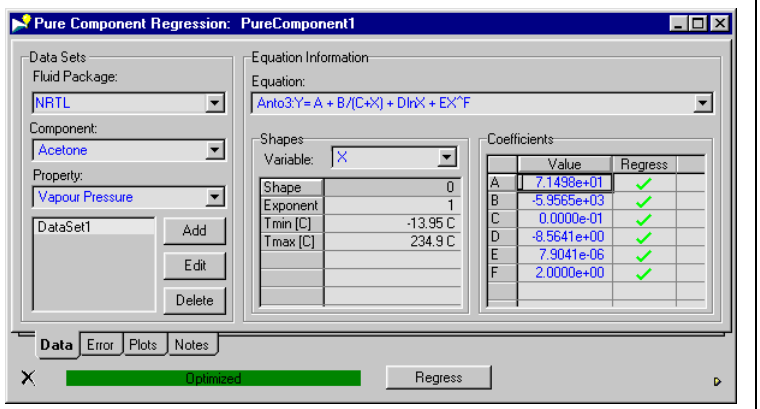
When you click the Regress button, the Pure Component Regression operation changes the values of the coefficients used to calculate the properties of the selected component.

# 4.2.1 Data Tab

The experimental data for the data set is entered in the Pure Component Data Set view. Refer to the **Pure Component Data Set View** section for more information.

The Data tab allows you to select the fluid package, component, property, and data set that will be used to generate new coefficient values.

**Figure 4.2**




The following table lists and describes the objects available in the Data tab:

| Object | Description |
|---|---|
| **Fluid Package drop-down list** | Allows you to select the fluid package that contains the components and property package you want to regress. |
| **Component drop-down list** | Allows you to select the component you want to regress. |
| **Property** | Allows you to select the property you want to regress. |
| **Data Sets list** | Displays the data sets available for the current operation. |
| **Add button** | Allows you to access the Pure Component Data Set view, which allows you to add a data set to the current operation. |
| **Edit button** | Allows you to edit the selected data set in the Data Sets list. Refer to the **Editing a Data Set** section for more information. |
| **Delete button** | Allows you to delete the selected data set from the Data Sets list. Refer to the **Deleting a Data Set** section for more information. |
| **Equation drop-down list** | Allows you to select an equation that will be used to calculate the selected property. |
| **Variable drop-down list** | Allows you to select a variable from the equation to observe its Shape information. |
| **Shapes table** | Displays the Shape information of the selected variable. |

Refer to the **Adding a Data Set** section for more information.

| Object | Description |
|---|---|
| **Coefficients table** | Displays the coefficients and their values from the selected equation. |
| **Value column** | Allows you to change the coefficient values. |
| **Regress column** | Allows you to toggle between keeping the coefficient value at the current setting or changing the coefficient value based on the regression results. |

A green checkmark indicates that the coefficient value is frozen.

A red cross indicates that the coefficient value is allowed to change.

# Adding a Data Set

To add a data set to the Pure Component Regression operation:

1. Open the Pure Component Regression view.
2. Click the **Data** tab.
3. Use the Fluid Package, Component and Property drop-down lists to select the fluid package, component, and property to be regressed.
4. Click the **Add** button. The Pure Component Data Set view appears.
5. Enter the experimental data for the data set.
6. When you are done entering the data, click the **Close** icon to close the Pure Component Data Set view.

Refer to the **Pure Component Data Set View** section for more information.

# Editing a Data Set

To edit a data set in the Pure Component Regression operation:

1. Open the Pure Component Regression view.
2. Click the **Data** tab.
3. In the Data Sets list, select the data set you want to edit.
4. Click the **Edit** button. The Pure Component Data Set view of the selected data set appears.
5. Edit the data set, then click the **Close** icon to close the Pure Component Data Set view.

# Deleting a Data Set

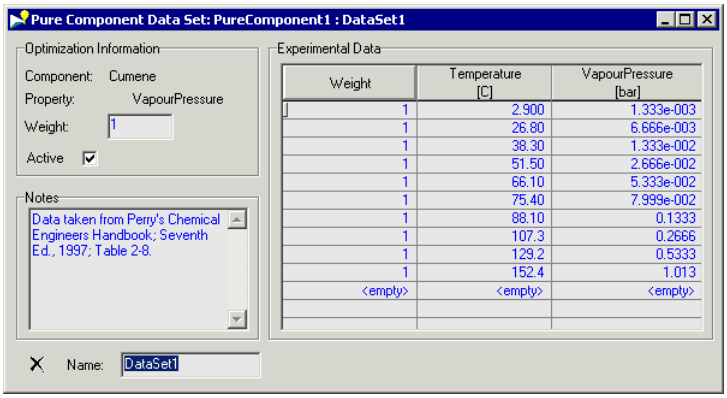
To delete a data set from the Pure Component Regression operation:

1. Open the Pure Component Regression view.
2. Click the **Data** tab.
3. In the Data Sets list select the data set you want to delete.
4. Click the **Delete** button.
5. Pure Component Regression will prompt you to confirm that you want to delete the data set from the operation.
   Click the **Yes** button to delete the data set, or click the **No** button to keep the data set.

# Pure Component Data Set View

The Pure Component Data Set view allows you to enter experimental data for the current data set.

**Figure 4.3**



The following table lists and describes the object available in the Pure Component Data Set view:

| Object | Description |
|---|---|
| **Optimization Information group** | Displays the selected component and property package associated with the current data set. |
| **Weight field** | Allows you to change the weight of the current data set. Refer to **Section 1.1.2 - Weighting** in the **Reference Guide** for more information. |
| **Active checkbox** | Allows you to toggle the calculation status of the current data set. |
| **Notes text editor** | Allows you to enter information about the current data set. |
| **Weight cell** | Allows you to specify the weight value for the experimental data. |
| **Temperature cell** | Allows you to specify the temperature value for the experimental data. |
| **Property cell** | Allows you to specify the selected property value for the experimental data. |
| **Delete icon** | Allows you to delete the current data set. |
| **Name field** | Allows you to change the name of the current data set. |

If the checkbox is checked, the current data set is included in the regression/ optimization calculation.

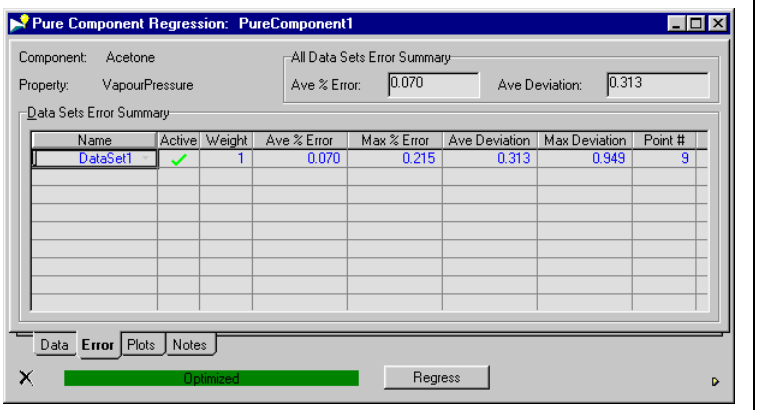
If the checkbox is unchecked, the current data set is removed from the regression/ optimization calculation.

Delete icon

# 4.2.2 Error Tab

The Error tab displays the summary information of the error/difference between the calculated data set values and the program's default values.

**Figure 4.4**




The following table lists and describes the objects available in the Error tab:

| Object | Description |
|---|---|
| **Ave % Error field** | Displays the calculated average percent error for all the entered data set. |
| **Ave Deviation field** | Displays the calculated average deviation for all the entered data set. |
| **Name cell** | Displays the name of all data sets for the current operation. |
| **Active checkbox** | Allows you to toggle the calculation status of the current data set. |
| **Weight cell** | Allows you to change the weight of the current data set. Refer to **Section 1.1.2 - Weighting** in the **Reference Guide** for more information. |
| **Ave % Error cell** | Displays the calculated average error between the data set and the default values. |
| **Max % Error cell** | Displays the calculated maximum error between the data set and the default values. |
| **Ave Deviation cell** | Displays the calculated average deviation between the data set and the default values. |
| **Max Deviation cell** | Displays the calculated maximum deviation between the data set and the default values. |
| **Point # cell** | Displays the number of experimental data points entered for the data set. |

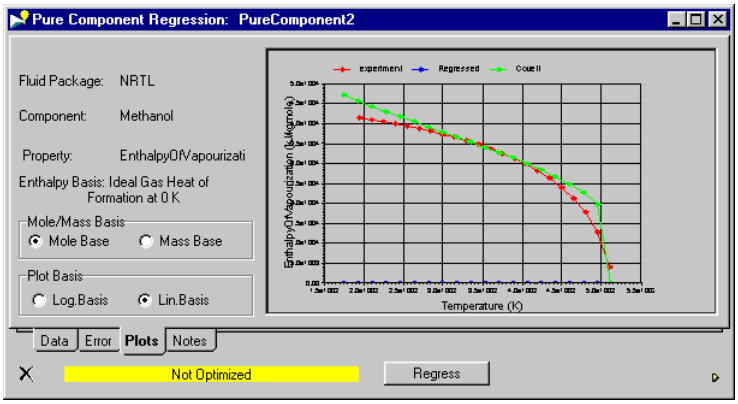
A green checkmark indicates that the current data set is included in the regression/optimization calculation.

A red cross indicates that, the current data set is not included in the regression/ optimization calculation.

# 4.2.3 Plots Tab

The Plots tab allows you to examine and compare the experimental data set values and the default values in a plot format.

**Figure 4.5**




The following table lists and describes the objects available in the Plots tab:

| Object | Description |
|---|---|
| **Mole/Mass Basis radio buttons** | Allows you to select the component basis type for the plot.<br>• Select the **Mole Base** radio button for a molar fraction.<br>• Select the **Mass Base** radio button for a mass fraction. |
| **Plot Basis radio button** | Allows you to select the plot type.<br>• Select the **Log Basis** radio button for a logarithm plot.<br>• Select the **Lin Basis** radio button for a linear plot. |

# 4.2.4 Notes Tab

The Notes tab allows you to:

- Change the name of the Pure Component Regression operation by entering a new name in the **Name** field.
- Enter information regarding the Pure Component Regression operation in the **Notes** text editor.

Any changes made to the information in the Notes text editor will appear in the text editor located at the bottom of the Thermodynamic Workbench Manager view when the Show Notes button has been clicked.

# 5 Fluid Phase Regression

# 5.1 Introduction

The Fluid Phase Regression operation allows you to derive interaction coefficients which are optimized for the process being considered.

By selecting appropriate data, you can fit interaction parameters at the temperature, pressure and range of compositions for your system and ensure better accuracy for a broader range of conditions.

There are software links to pure and multi-component data banks and facilities to import experimental plant data. The program includes the TRC VLE and VLLE experimental data bank.

## Technical Capabilities

The following is a list of the technical capabilities of the Fluid Phase Regression operation:

- There are seventeen objective functions to choose from, including bubble temperature, bubble pressure and relative volatility. This ensures that coefficients are generated that meet your process requirements.
- Thirteen different data types for regression are accepted. A regression scenario can contain several sets of data, each of a different type and each using a different objective function and weighting.
- The Consistency Test allows you to examine the thermodynamic consistency of experimental data.
- The Error tables and plots allow you to generate a table or plot for each data set.
- Experimental data can be plotted against calculated points to visually examine the fit.

There are three locations where you can change the weight of the data set:

- On the Fluid Phase Regression view, Summary tab, Weight In Experiment field.
- On the Fluid Phase Regression view, Errors tab, Weight cell.
- On the Fluid Phase Data Set view, Basic Data tab, Weight field.

# 5.2 Fluid Phase Regression View

The Fluid Phase Regression operation allows you to take experimental data specifically chosen for the system conditions and regress them to new interaction parameters using the previous mentioned thermodynamics model.

The default interaction parameters are usually reliable, although it is important to ensure that they were regressed under conditions similar to the current conditions.

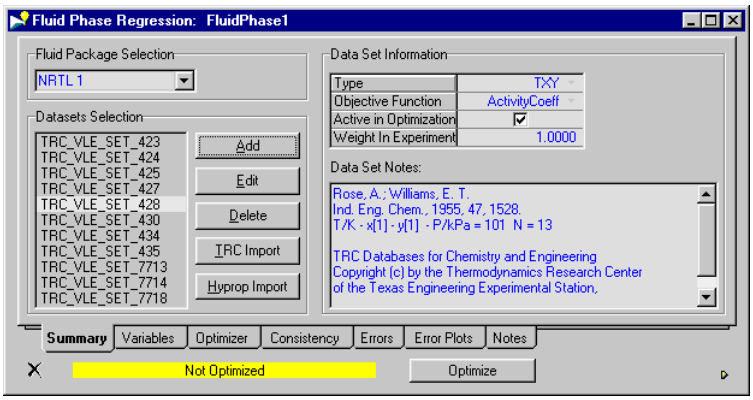
The default interaction parameters are located in the Fluid Package view, Binary Coefficients tab. Refer to **Section 9.3.3 - Binary Coefficients Tab** from the **User Guide** for more information.

To access a Fluid Phase Regression operation:

- From the **Feature** menu, select **Fluid Phase Regression**.
- From the **Managers** menu, select **Thermodynamic Workbench Manager.** The manager view appears. In the left list, select **FluidPhaseRegression**, then click the **Add** button.

To access previously created Fluid Phase Regression operations, refer to **Section 1.2.2 - Editing an Operation**.

**Figure 5.1**




Interaction parameters can be regressed from multiple data sets. In the above view, TRC sets with TXY data have been imported. Data Set Notes text editor show the source of the data.

The Fluid Phase Regression view contains seven tabs: Summary, Variables, Optimizer, Consistency, Errors, Error Plots, and Notes. The view also contains four objects at the bottom of the view.

The following table lists and describes each object at the bottom of the view.

| Object | Icon | Description |
|---|---|---|
| **Delete icon** |  | Allows you to delete the selected Fluid Phase Regression operation. |
| **Status bar** | | Displays the status of the selected Fluid Phase Regression operation. |
| **Optimize button** | | Allows you to regress the interaction parameters based on the experiment data values from the selected data set.<br>Before running the optimizer, set the view so you can observe the solution progress; Optimizer or Variables tab is recommended. Ensure the Parameters radio button is selected on the Variables tab. It is probably most useful to observe the $a_{ij}$ parameters. |
| **Open... Window icon** |  | Allows you to open the active tab as a separate view. |

It is recommended that you check how well the experimental data matches the calculated data based on the default interaction parameters before optimizing the data.

**The optimized value of the binary interaction parameters (BIP) depends upon the initial guesses (previous BIP values), so it is possible to get different BIP values every time you click the Optimize button.**

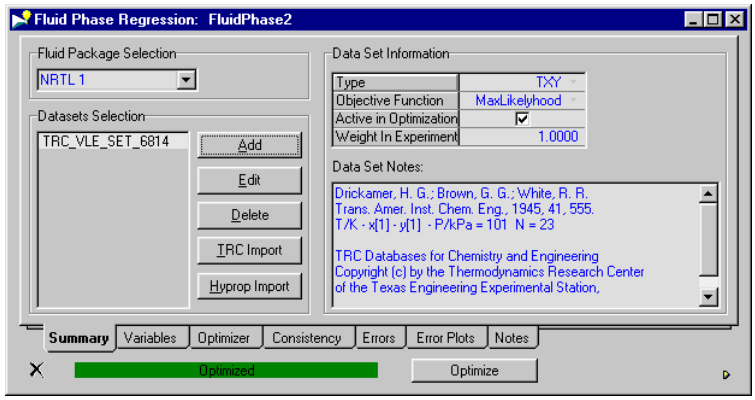
**For this reason, it is important to examine the plots and error values to determine how well the calculated parameters match the experimental values and which data set you prefer to use.**

The following sections describes in detail each tab in the Fluid Phase Regression view.

# 5.2.1 Summary Tab

The Summary tab allows you to manipulate experimental data in a data set. The experimental data values can be entered manually, or can be automatically selected from data sets in the TRC libraries of Vapour Liquid Equilibrium, Liquid Liquid Extraction, and Heats of Mixing data. The TRC database contains data for more than 16000 fitted binaries.

**Figure 5.2**




The following table lists and describes each object in the Summary tab:

| Object | Description |
|---|---|
| **Fluid Package Selection drop-down list** | Allows you to select the fluid package you want to analyze. |
| **Datasets Selection list** | Displays the list of data sets available for the current Fluid Phase Regression operation. |
| **Add button** | Allows you to create a data set and manually add experiment data values to the data set. See the **Entering Values for a Data Set** section for more information. |
| **Edit button** | Allows you to edit the selected data set. See the **Editing a Data Set** section for more information. |
| **Delete button** | Allows you to delete the selected data set. See the **Deleting a Data Set** section for more information. |
| **TRC Import button** | Allows you to import data sets from the TRC database. See the **Importing Data from TRC Database** section for more information. |
| **Hyprop Import button** | Allows you to import data sets from Hyprop *.set files. See the **Importing Data from a Hyprop File** section for more information. |

| Object | Description |
|---|---|
| **Type cell** | Allows you to select the type of data set you want to analyze. |
| **Objective Function cell** | Allows you to select different objective functions to minimize the error. See the **Objective Functions** section for more information. |
| **Active in Optimization checkbox** | Allows you to toggle the calculation status of the current data set. |
| **Weight in Experiment cell** | Allows you to "distort" the fit of the data set in order to better represent the behaviour of a specific region. Refer to **Section 1.1.2 - Weighting** in the **Reference Guide** for more information. |
| **Data Sets Notes text editor** | Displays the notes that describes the selected data set and allows you to modify the notes. |

If the checkbox is checked, the current data set is included in the regression/ optimization calculation.

If the checkbox is unchecked, the current data set is removed from the regression/ optimization calculation.

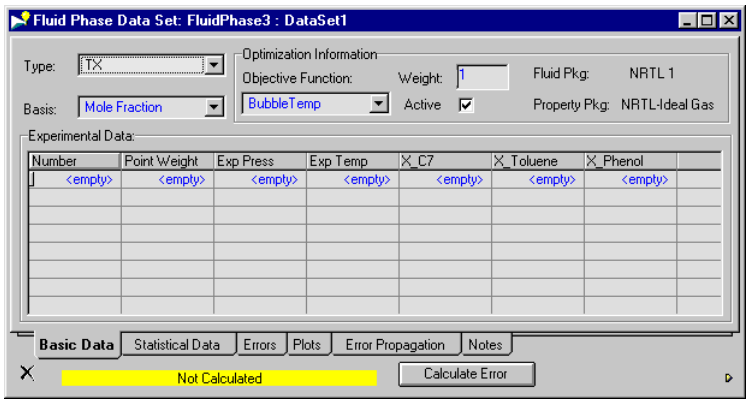
# Entering Values for a Data Set

To manually enter the experimental data:

1. Open the Fluid Phase Regression view.
2. Click the **Summary** tab.
3. In the Fluid Package Selection drop-down list, select a fluid package.
4. In the Datasets Selection group, click the **Add** button. The Fluid Phase Data Set view appears.

For more information on the Fluid Phase Data Set view, refer to **Section 5.3 - Fluid Phase Data Set View**.

**Figure 5.3**




5. In the **Basic Data** tab, use the Type drop-down list to select the type of data set you are entering.

6. Use the Basis drop-down list to select the basis fraction type for the experimental data. There are three types: Mole Fraction, Mass Fraction, and Volume Fraction.
7. In the Optimization Information group, select the objective function, specify the weight, and indicate if you want the data set to be active in the current operation calculations.

Click the **Calculate Error** button at the bottom of the view to calculate the deviation between the plot and experiment data values.

8. In the Experimental Data table, enter values for the data set.
9. When you have finished entering the experimental data, click the **Close** icon to close the Fluid Phase Data Set view.

# Importing Data from TRC Database

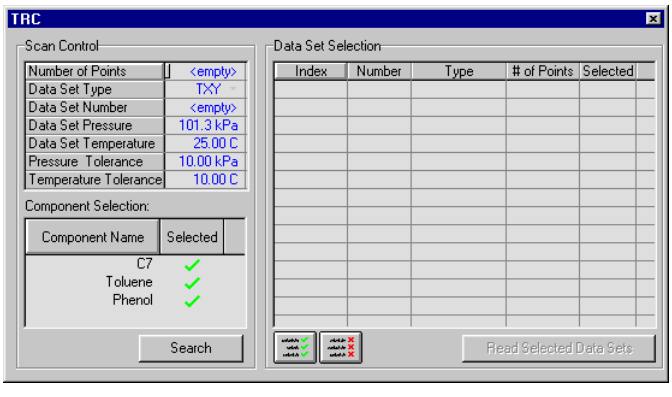
To import experimental data from the TRC libraries:

1. Open the Fluid Phase Regression view.
2. Click the **Summary** tab.
3. In the Fluid Package Selection drop-down list, select a fluid package.

For more information on the TRC view, refer to **Section 5.4 - TRC View**.

4. Click the **TRC Import** button in the Datasets Selection group. The TRC view appears.

**Figure 5.4**




A red cross indicates that the component is not selected.

A green checkmark indicates that the variable is selected.

To find all data set types, select the All Data option from the Data Set Type drop-down list.

5. On the TRC view, use the filter options in the Scan Control table to find the required data sets.
6. In the Component Selection table, select the two components required for the data set by checking or unchecking the icons beside the components.

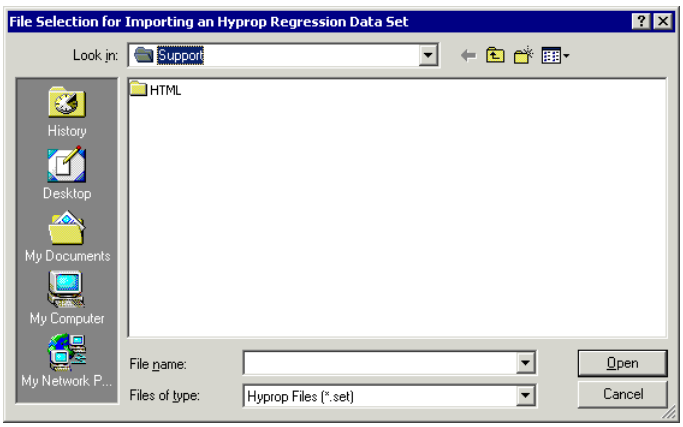
7. Click the **Search** button to find all the data sets for the selected two components. The list of data sets appear in the Data Set Selection table.
8. Click in the **Selected** column beside the required data set to select it for import.
9. After selecting all the data sets you want, click the **Read Selected Data Sets** button.
   The TRC view closes and the selected data sets appear in the Datasets Selection list on the **Summary** tab of the Fluid Phase Regression view.

# Importing Data from a Hyprop File

To import data from a Hyprop file:

1. Open the Fluid Phase Regression view.
2. Click the **Summary** tab.
3. In the Fluid Package Selection drop-down list, select a fluid package.
4. In the Datasets Selection group, click the **Hyprop Import** button.
   The File Selection view appears.

**Figure 5.5**




5. Use the Look in drop-down list to find the *.set file that contains the data set you require.
6. Select the file, then click the **Open** button.

7. The File Selection view closes and the data set from the selected file appears in the Datasets Selection list on the **Summary** tab of the Fluid Phase Regression view.

# Editing a Data Set

To edit a data set already selected for the operation:

1. Open the Fluid Phase Regression view.
2. Click the **Summary** tab.
3. In the Datasets Selection list, select the data set you want to edit.
4. Click the **Edit** button. The Fluid Phase Data Set view appears.
5. Edit the information as required.
6. When you are finished, click the **Close** icon to close the view.

# Deleting a Data Set

To delete a data set for the operation:

1. Open the Fluid Phase Regression view.
2. Click the **Summary** tab.
3. In the Datasets Selection list, select the data set you want to edit.
4. Click the **Delete** button.
   You will be prompt to confirm that you want to delete the data set from the operation.
5. Click the **Yes** button to delete the data set, or click the **No** button to keep the data set.

# Objective Functions

Since the ability of thermodynamic models to predict all the properties accurately is limited, it is possible to choose which thermodynamic property will be represented with the best possible accuracy. A fairly straight-forward way of doing this mathematically is through the use of objective functions, each tailor-made to represent a specific property.

## Objective Function Type

The objective functions available in the drop-down list depends on the data set type.

You can select the objective function from two locations:

- On the Fluid Phase Regression view, **Summary** tab, **Objective Function** drop-down list.
- On the Fluid Phase Data Set view, **Basic Data** tab, **Objective Function** drop-down list.

Your choice of objective function will control the variable(s) to which the error function will be minimized. All of the objective function types are listed in the following table.

| Objective Function | Description |
|---|---|
| **Bubble Temperature** | Minimize with respect to the measured bubble temperature. This method is useful when you want to predict the bubble point temperature of the system as accurately as possible, and is particularly useful when modeling evaporators. |
| **Bubble Pressure** | Minimize with respect to the measured bubble pressure. This method is useful for the design of relief systems, where the knowledge of accurate saturation pressures is necessary. |
| **Liquid Composition** | Minimize with respect to the measured liquid composition (performs a dew point calculation). This method is useful when you want the composition of the liquid to be simulated as accurately as possible. |
| **Vapour Composition** | Minimize with respect to the measured vapour composition (performs a bubble point calculation). This method is useful when you want the composition of the vapour to be simulated as accurately as possible. |
| **Maximum Likelihood** | Minimize with respect to the maximum likelihood function. This is a simultaneous minimization of bubble temperature, vapour composition, dew point and liquid composition. Although it is the most rigorous objective function from a statistical point of view, it is also the one that is most computer intensive, and the improvement upon simpler objective functions is not always evident. |
| **Liq&Vap Composition** | Minimize with respect to the measured liquid and vapour composition. |
| **Activity Coefficient** | Minimize with respect to the components' activity coefficients. This is the default function for the activity models and it combines the combining of the error in the liquid phase with a fairly rapid convergence rate. Also, it is very useful when regressing data reported as infinite dilution activity coefficients. Equations of State can use this objective function, but the results tend to be mediocre for highly polar systems. |
| **Fugacity** | Minimize with respect to the equality of fugacities in the vapour and liquid phases. This is the standard objective function when working with Equations of State. It combines the vapour and liquid in one unique function and is generally adequate to give a reasonable representation of the VLE behaviour of most systems. |
| **Separation Factor** | Minimize with respect to the separation factor (for liquid-liquid equilibrium problems). Useful for liquid-liquid problems such as an extractor or decanter in an azeotropic dehydration tower. |
| **K-factor** | Minimize with respect to the components k-factors (y/x). This method is useful for systems that have comparable k-factors for all the components. |
| **Log (K-factor)** | Minimize with respect to the natural logarithm of k-factors. This is useful for systems with one or more components for which the k-factor has a very different order of magnitude in comparison with the other components in the system. It is usually used for gas absorption problems. |

| Objective Function | Description |
|---|---|
| **Relative Volatility** | Minimize with respect to the relative volatility (volatility of component *i* over the volatility of the last component). This is useful for systems that have comparable relative volatilities, like propane/propylene or ethane/ethylene splitters. |
| **Log (Relative Volatility)** | Minimize with respect to the natural logarithm of the relative volatility of component *i*. This is useful for systems with one or more components for which the relative volatility has a very different order of magnitude in comparison with the other components in the mixture. |
| **K-factor & Vap. Composition** | Minimize with respect to the k-factor and vapour composition. |
| **Volatility & K-factor** | Minimize with respect to the relative volatility and k-factor. This is useful when the behaviour of the component that makes up the majority of the vapour phase is of greater interest. |
| **Log(Volatility) & Log(K-factor)** | Minimize with respect to the natural log of the relative volatility and natural log of the k-factor. |
| **TXXY Bubble Temperature** | Minimize with respect to the Bubble Temperature of a 2-liquid/vapour system. |
| **TXXY Bubble Pressure** | Minimize with respect to the Bubble Pressure of a 2-liquid/vapour system. |
| **Dew Temperature** | Minimize with respect to the measured dew temperature. This method is useful when you want to predict the dew point temperature of the system as accurately as possible. |
| **Dew Pressure** | Minimize with respect to the measured dew pressure. This method is useful when it is desired to predict the dew pressure of the system as accurately as possible. |
| **Solubility 1 $\rightarrow$ 2** | This method optimizes the solubility of component 1 in component 2 (valid only for binary systems). It is useful when modeling water decontamination systems. |
| **Excess Enthalpy** | Minimize with respect to the enthalpy of mixing. |

## Objective Function Availability

Each data set can utilize only a specific set of objective functions. The objective functions available for each type of data set are listed below:

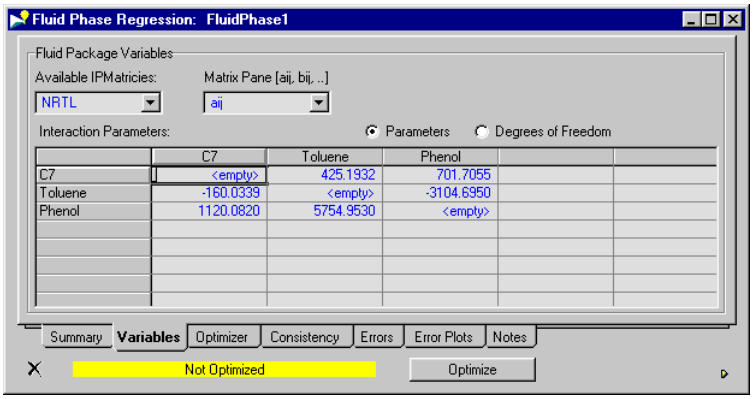
| Data Set | Available Objective Functions |
|---|---|
| **TX** | Bubble Temperature, Bubble Pressure |
| **TY** | Dew Temperature, Dew Pressure |
| **PX** | Bubble Temperature, Bubble Pressure |
| **PY** | Dew Temperature, Dew Pressure |
| **TPX** | Bubble Temperature, Bubble Pressure |
| **PXY** | All except Dew Temperature, Dew Pressure, Separation Factor, Solubility $1 \rightarrow 2$ , Excess Enthalpy |
| **TXY** | All except Dew Temperature, Dew Pressure, Separation Factor, Solubility $1 \rightarrow 2$ , Excess Enthalpy |
| **TXX** | Separation Factor |
| **TPXY** | All except Dew Temperature, Dew Pressure, Separation Factor, Solubility $1 \rightarrow 2$ , Excess Enthalpy |
| **Gamma** | Activity Coefficient |

| Data Set | Available Objective Functions |
|---|---|
| **Solubility** | Solubility $1 \rightarrow 2$ |
| **Excess Enthalpy** | Excess Enthalpy |
| **TXXY** | TXXY Bubble Temperature, TXXY Bubble Pressure |

# 5.2.2 Variable Tab

The Variables tab in the Fluid Phase Regression view is similar to the Binary Coefficient tab of the Fluid Package view.

**Figure 5.6**




If you have not optimized the binary interaction parameter value, the values appearing in the Interaction Parameters matrix are the default values set in the Fluid Package view, Binary Coefficients tab.

The binary interaction parameter values displayed in the Interaction Parameters matrix changes when you optimize the values based on the selected data set.

The following table lists and describes the objects in the Variables tab:

| Object | Description |
|---|---|
| **Available IPMatricies drop-down list** | Allows you to select the model used to calculate the fluid behaviour. The models available will depend on the type of property package selected. |
| **Matrix Pane drop-down list** | Allows you to select different coefficient variables of the model to manipulate. The number of coefficient variables varies depending on the model selected. |
| **Parameters radio button** | When selected, this options allows you to see the binary interaction parameter values in the matrix. |

| Object | Description |
|---|---|
| **Degrees of Freedom radio button** | When selected, this option allows you to lock, glue, or free the interaction parameter values in the matrix. Refer to the **Changing the Freedom of the Binary Interaction Parameter** section for more information. |
| **Interaction Parameters matrix** | Displays the binary interaction values of the selected coefficient variables associated with the selected models. |

For more information regarding the binary interaction matrix, refer to **Section 9.3.3 - Binary Coefficients Tab** in the **User Guide**.

## Changing the Freedom of the Binary Interaction Parameter

To change the status of the binary interaction parameter value:

1. Open the Fluid Phase Regression view.
2. Click the **Variables** tab.
3. Click the **Degrees of Freedom** radio button.
4. In the Interaction Parameters table, select the cell containing the binary interaction parameter that you want to change.
5. Click the down arrow in the cell to open the drop-down list.
6. In the drop-down list, select the required status for the interaction parameter.

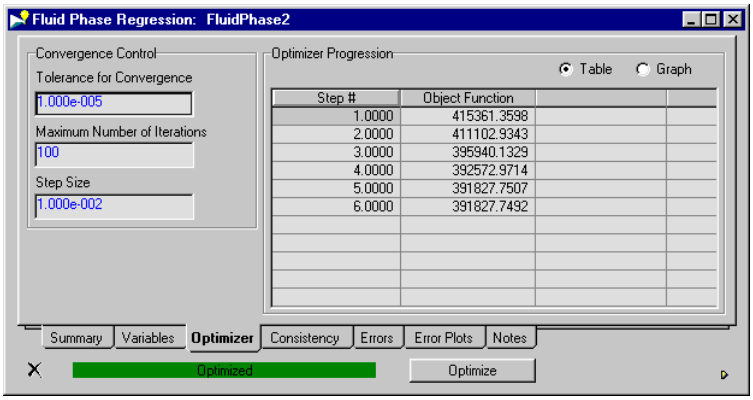
There are three options for the binary interaction parameter freedom status:

- Locked. Freezes the current value for the parameter so the value does not change even after applying the Optimization command.
- Glued. Ensures that the pair of parameters are the same (e.g., parameter $b_{ji} = b_{ij}$).
- Free. Allows the program to change the value in the parameter when applying the Optimization command.

# 5.2.3 Optimizer Tab

The Optimizer tab contains the convergence control options used when calculating the new value for the binary interaction parameter based on the selected data set.

**Figure 5.7**




The following table lists and describes the objects in the Optimizer tab:

| Object | Description |
|---|---|
| **Tolerance for Convergence field** | Allows you to specify the tolerance value for the convergence calculation during optimization. |
| **Maximum Number of Iterations field** | Allows you to specify the maximum number of iterations performed during calculation. |
| **Step Size field** | Allows you to specify the step size of the iteration during calculation. |
| **Optimizer Progression Table/Plot** | Displays the progress of the optimization calculation in a table or plot format.<br>The table or plot is blank when 'Not Optimized' appears in the status bar. |
| **Table radio button** | Allows you to see the progress of the optimization calculation in a table format. |
| **Graph radio button** | Allows you to see the progress of the optimization calculation in a plot format. |

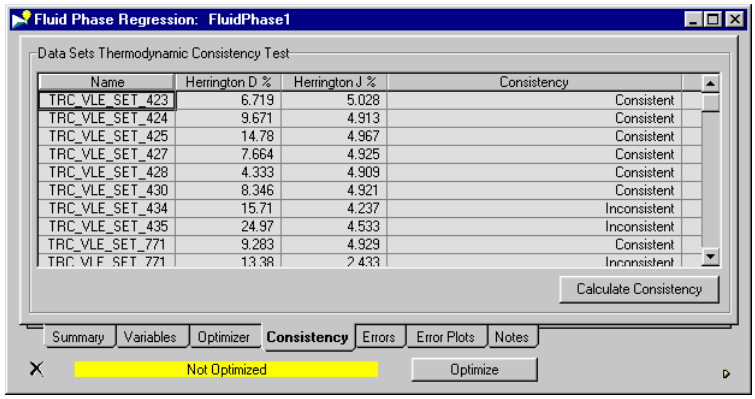
For more information on manipulating the plot, refer to **Section 8.2 - Graph Control View** in the **User Guide**.

# 5.2.4 Consistency Tab

Click the **Calculate Consistency** button to activate the consistency test.

The Consistency tab allows you to verify if the data set values are consistent.

**Figure 5.8**




Fluid Phase Regression uses the Herrington Consistency test equation to test the consistency of the data set.

The Herrington Consistency test confirms that the isothermal, isobaric Gibbs-Duhem equation is satisfied.

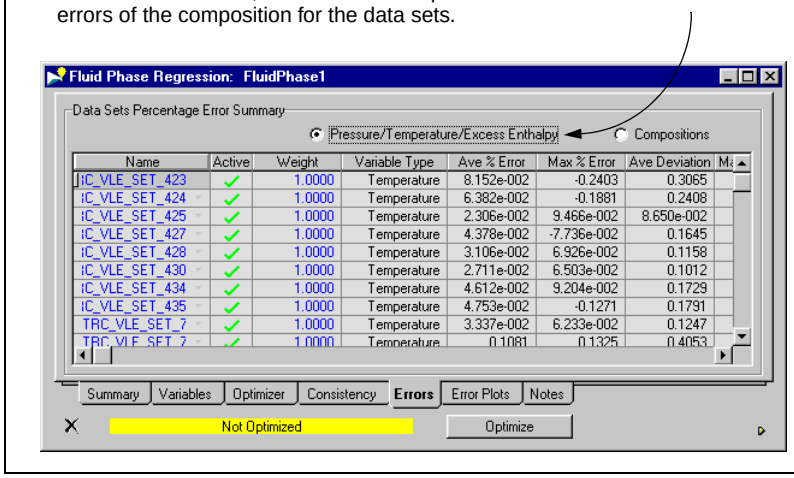
For more information regarding the Herrington consistency text, refer to **Section 1.1.4 - Herrington Consistency Test Equations** in the **Reference Guide**.

If the Herrington D value is $\leq 5\%$ at constant temperature, the data is considered consistent. Similarly, if the Herrington J value - Herrington K value is $\leq 10\%$ at constant pressure, the data is considered consistent (Gmehling and Onken, 1977[54])

# 5.2.5 Errors Tab

The Errors tab displays the average errors and deviation between the experimental data and the calculated data of the data sets in a table format.

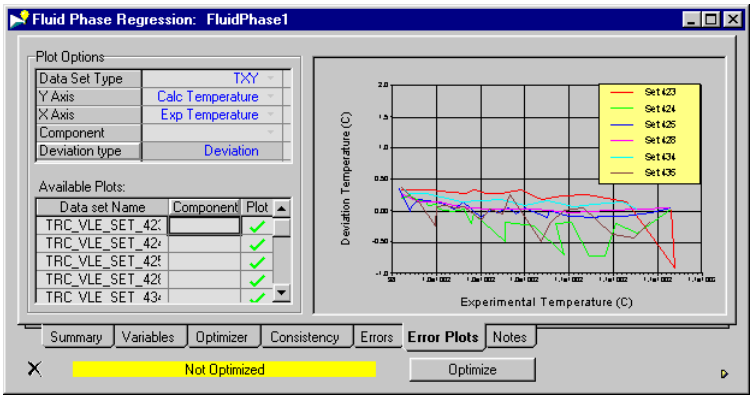
**Figure 5.9**



# 5.2.6 Error Plots Tab

The Error Plots tab displays the errors and deviations between the experimental data and the calculated data of the data sets in a plot format.

**Figure 5.10**




The following table lists and describes the objects available in the Error Plots tab:

| Object | Description |
|---|---|
| **Data Set Type drop-down list** | Allows you to select the data set type you want to appear on the plot. |
| **Y Axis drop-down list** | Allows you to select the calculated variable that appears on the Y axis of the plot. The following is a list of all the variables available for the Y axis:<br>• Calculated Temperature<br>• Calculated Pressure<br>• Calculated Vapour Composition<br>• Calculated Activity Coefficient<br>• Calculated K Factor<br>• Calculated Relative Volatility |
| **X Axis drop-down list** | Allows you to select the experimental variable that appears on the X axis of the plot. The following is a list of all the variables available for the X axis:<br>• Experimental Temperature<br>• Experimental Pressure<br>• Experimental Liquid Composition<br>• Experimental Vapour Composition |

The selections available in the Y and X axis drop-down lists depend on the data set type selected.

| Object | Description |
|---|---|
| **Component drop-down list** | Allows you to select the component that will appear in the plot. Available only when the Calculated Vapour Composition variable is selected for the Y axis. |
| **Deviation Type drop-down list** | Allows you to select the deviation type value that will appear on the plot. |
| **Available Plots table** | Allows you to select which data set you want to see on the plot. The data set available in the list depends on the selected data set type and the selected variables for the plot axes. |
| **Plot** | Displays a plot based on the options selected in the Plot Options group. |

For more information on manipulating the plot, refer to **Section 8.2 - Graph Control View** in the **User Guide**.

## 5.2.7 Notes Tab

The Notes tab allows you to:

- Change the name of the Fluid Phase Regression operation by entering a new name in the **Name** field.
- Enter information regarding the Fluid Phase Regression operation in the **Notes** text editor.

Any changes made to the information in the Notes text editor will appear in the text editor located at the bottom of the Thermodynamic Workbench Manager view when the Show Notes button has been clicked.

# 5.3 Fluid Phase Data Set View

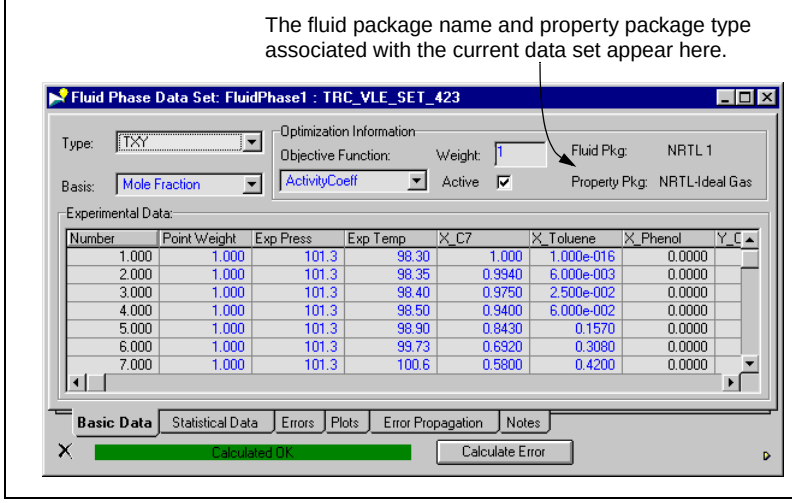
The Fluid Phase Data Set (FPDS) view contains individual data set information as supplied by the user or imported from the TRC database.

To access FPDS view:

1. Open the Fluid Phase Regression view.
2. Click the **Summary** tab.
3. From the Datasets Selection list, select the data set you want to view.
4. Click the **Edit** button. The FPDS view appears for the selected data set.

You can also double-click the data set in the Datasets Selection list to open the FPDS view.

**Figure 5.11**




The Fluid Phase Data Set view contains six tabs: Basic Data, Statistical Data, Errors, Plots, Error Propagation, and Notes. The view also contains four objects at the bottom of the view. The following table lists and describes the objects available in this view.

| Object | Icon | Description |
|---|---|---|
| **Delete icon** | | Allows you to delete the selected Fluid Phase Data Set. |
| **Status bar** | | Displays the status of the selected Fluid Phase Data Set. |

The Errors and Plots tabs contain no relevant information until you click the Calculate Error button.

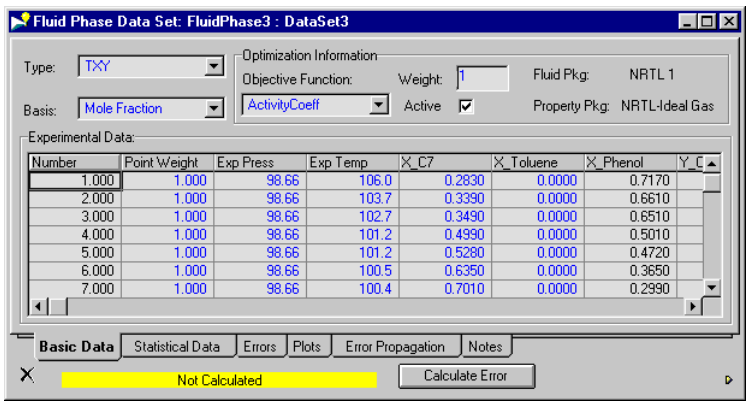
| Object | Icon | Description |
|---|---|---|
| **Calculate Error button** | | Allows you to calculate the error between the experimental data and the calculated data. |
| **Open Page as Separate Window icon** |  | Allows you to open the active tab as a separate view. |

The following sections describes in detail each tab in the Fluid Phase Data Set view.

# 5.3.1 Basic Data Tab

The Basic Data tab allows you to enter all the basic information for creating a data set.

**Figure 5.12**




The following table lists and describes the objects in the Basic Data tab:

If you change the data set type, the current data in the data set will be deleted.

| Object | Description |
|---|---|
| **Type drop-down list** | Displays the data set type for the active data set. You can also change the data set type for the active data set using this drop-down list. |
| **Basis drop-down list** | Allows you to select the basis fraction of the data values in the Experimental Data table. |
| **Objective Function drop-down list** | Allows you to select different objective functions to minimize the error. See the **Objective Functions** section for more information. |

| Object | Description |
|---|---|
| **Weight field** | Allows you to 'distort' the fit of the data set in order to better represent the behaviour of a specific region. Refer to **Section 1.1.2 - Weighting** in the **Reference Guide** for more information. |
| **Active checkbox** | Allows you to toggle the calculation status of the current data set. |
| **Experimental Data table** | Allows you to see and/or manipulate the experimental data for the active data set. The columns available in the table vary depending on the selected data set type. |

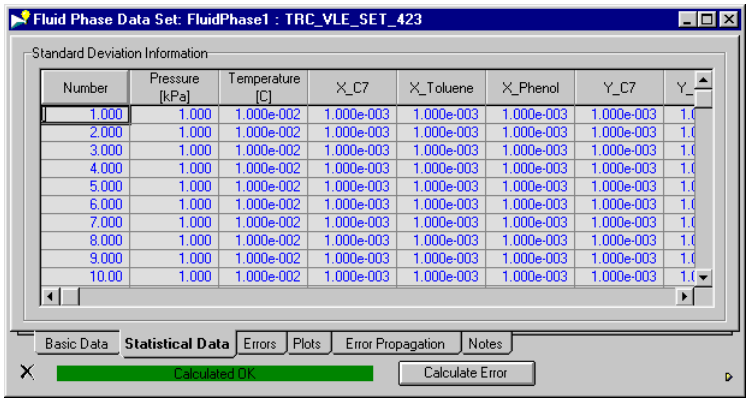
If the checkbox is checked, the current data set is included in the regression/ optimization calculation.

If the checkbox is unchecked, the current data set is removed from the regression/ optimization calculation.

# 5.3.2 Statistical Data Tab

The Statistical Data tab displays the standard deviation information for the current data set.

**Figure 5.13**

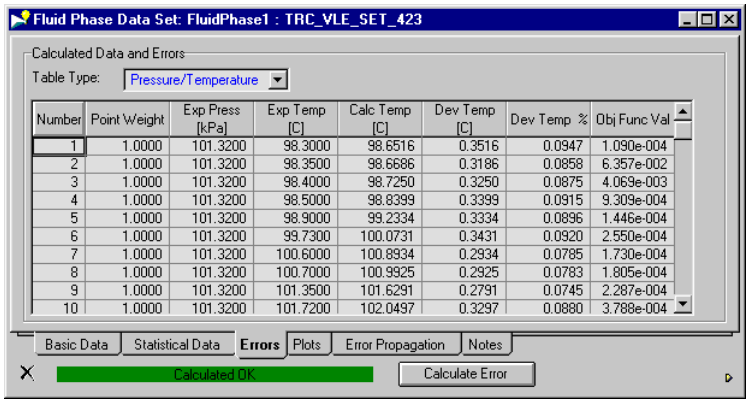


# 5.3.3 Errors Tab

The Calculated Data of Errors table will appear blank if Not Calculated appears in the status bar.

The Errors tab displays the error/deviation values between the experiment data points and the calculated data points in a table format.

**Figure 5.14**




The Table Type drop-down list allows you to select other error values. The error values available are:

- Pressure/Temperature
- Vapour Composition
- Activity Coefficients
- KFactor
- Relative Volatility

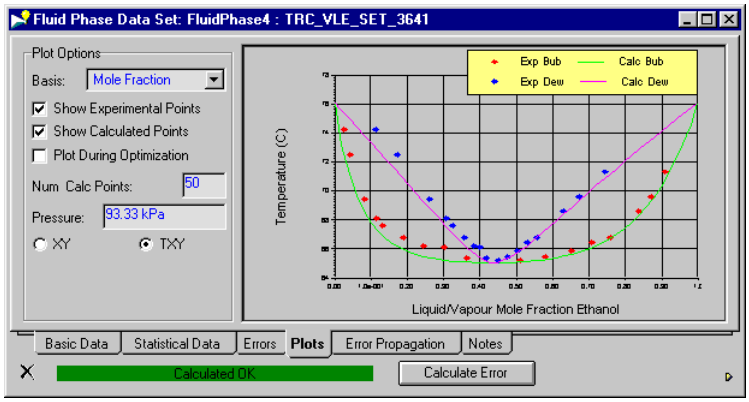
The Table Type drop-down list is only available for TXY and PXY data set types.

# 5.3.4 Plots Tab

The plot will appear blank if Not Calculated appears in the status bar.

The Plots tab allows you to view the plots created by the experimental data in the data set and the calculated data based on the binary interaction parameter values. The plots allow you to compare how well the calculated values fit the experimental values.

**Figure 5.15**




The following table lists and describes the objects available in the Plots tab:

For the calculated data points, the program automatically connects the points with a plot line.

| Object | Description |
|---|---|
| **Basis drop-down list** | Allows you to set the basis fraction in the plot as mole fraction, mass fraction, or volume fraction. |
| **Show Experiment Points checkbox** | Allows you to show or hide the experiment data points on the plot.<br>Check the checkbox to show the data points, or uncheck the checkbox to hide the data points. |
| **Show Calculated Points checkbox** | Allows you to show or hide the calculated data points on the plot.<br>Check the checkbox to show the data points, or uncheck the checkbox to hide the data points. |
| **Plot During Optimization checkbox** | Allows you to toggle between showing or hiding the changes in data in the plot when the optimization calculations are being performed. |
| **Num Calc Points field** | Allows you to specify the number of calculated data points on the plot. |
| **Pressure field** | Allows you to change the pressure value used to calculate the data points. |

| Object | Description |
|---|---|
| **XY / TXY radio button** | Allows you to toggle between the Vapour Fraction vs. Liquid Fraction plot (XY) and the Temperature vs. Vapour/ Liquid Fraction plot (TXY). |
| **Plot** | Displays the plot based on the selected options in the Plot Options group.<br>To access more plot options, right-click anywhere in the plot to open the Object Inspect menu. |

Refer to **Section 7.4 - Plot Area** in the **User Guide** for more information regarding the plot options in the Object Inspect menu.

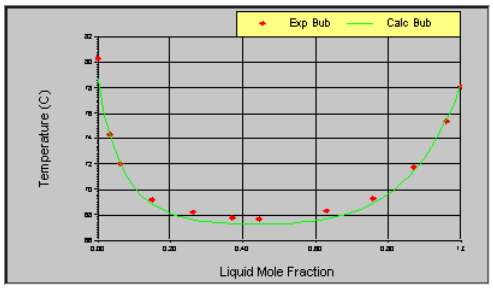
# Data Set Plots

The following sections list the types of data set plots available. The type of plot that appears depends on the option you select in the Type drop-down list on the Basic Data tab of the Fluid Phase Data Set view.

## TX Data Set

The calculated line is generated by performing a series of bubble point calculations at a fixed pressure from compositions ranging from 0.0 to 1.0. Since this is a TX data set, the pressure should be constant for all the data points.

**Figure 5.16**

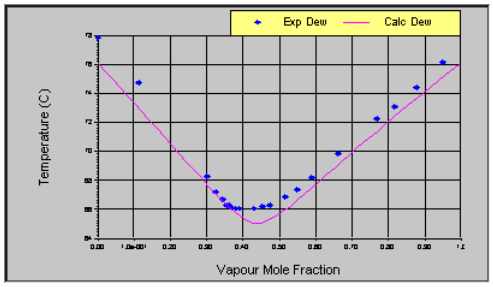



TX Data Set (Benzene/Ethanol)

## TY Data Set

The calculated line is generated by performing a series of dew point calculations at a fixed pressure from compositions ranging from 0.0 to 1.0. Since this is a TY data set, the pressure should be constant for all the data points.

**Figure 5.17**

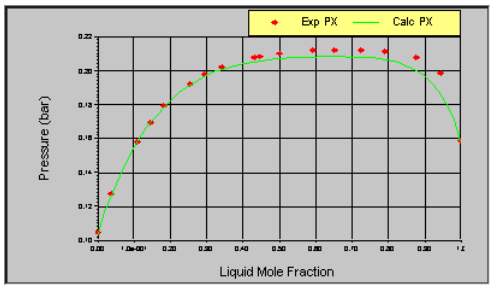



TY Data Set (Benzene/Ethanol)

## PX Data Set

The calculated line is generated by performing a series of bubble point calculations at fixed temperature from compositions ranging from 0 to 1.0. Since this is a PX data set, the temperature should be constant for all data points.

**Figure 5.18**

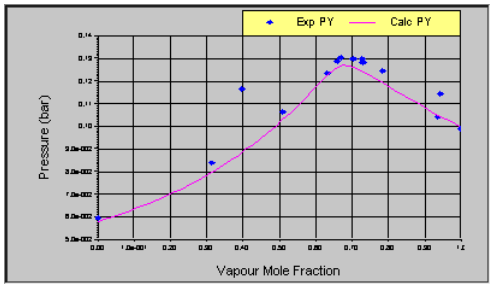



PX Data Set (Benzene/Ethanol)

## PY Data Set

The calculated line is generated by performing a series of dew point calculations at fixed temperature from compositions ranging from 0.0 to 1.0. Since this is a PY data set, the temperature should be constant for all data points.

**Figure 5.19**




PY Data Set (Benzene/Ethanol)

## TPX Data Set

The calculated data points are bubble temperatures determined using the input composition and pressure for each data point.

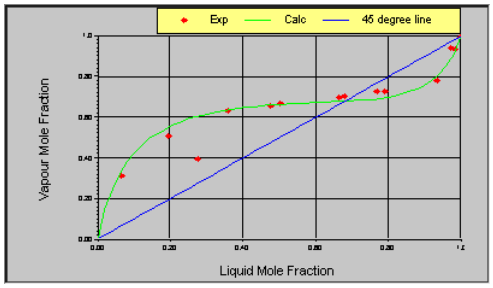
**The calculated line between data points is not generated because the pressure may not be the same for all points.**

# PXY Data Set

## XY Radio Button

The calculated line is generated by performing a series of bubble point calculations for compositions ranging from 0.0 to 1.0 using the temperature of the first data point. For a PXY data set the temperature should be constant.

**Figure 5.20**

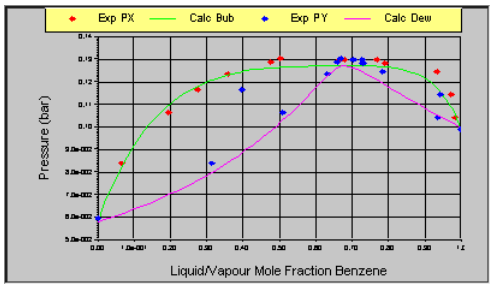



PXY Data Set (Benzene/Ethanol)
XY radio button selected

### PXY Radio Button

The calculated lines are generated by performing a series of bubble and dew point calculations given the temperature, which for PXY should be constant.

**Figure 5.21**



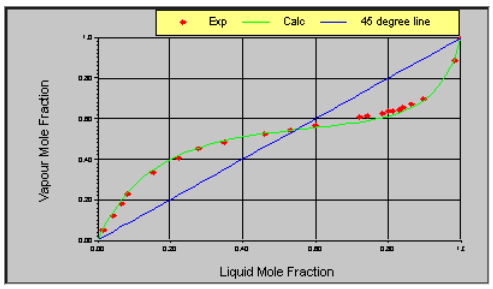

PXY Data Set (Benzene/Ethanol)
PXY radio button selected

## TXY Data Set

### XY Radio Button

The calculated line is generated by calculating the bubble point temperatures for liquid compositions ranging from 0.0 to 1.0. For TXY, the pressure is constant.

**Figure 5.22**

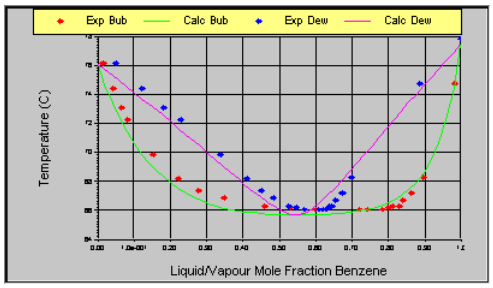



TXY Data Set (Benzene/Ethanol)
XY radio button selected

### TXY Radio Button

The lines are generated by calculating the bubble and dew temperatures using the pressure from the first data point and plotting the bubble and dew temperature curves. The pressure should be constant.

**Figure 5.23**




TXY Data Set (Benzene/Ethanol)
TXY radio button selected

## TPXY Data Set

The data points are bubble temperatures calculated using the user supplied composition and pressure for each data point.

**No calculated line can be generated because the pressure for each data point might change.**

## TXX Data Set

Each calculated point is determined by creating a feed for the flash equal to the arithmetic average of the composition of light and heavy phases, and performing a bubble temperature calculation at the pressure of the first data point (in a TXX data set the pressure should be constant). The obtained temperature vs. the light and heavy liquid compositions of component 1 is plotted.

## Activity Coefficient Data Set

Each calculated activity coefficient curve is generated using mole fractions ranging from 0.0 to 1.0 and the pressure of the first data point, performing a bubble temperature calculation. The activity coefficient is always calculated for the first liquid phase.

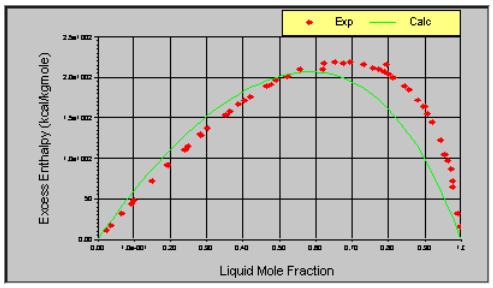
## Solubility Data Set

Each calculated data point is the value of the square root of the objective function value for the point plus the value of the data point.

## Excess Enthalpy Data Set

The continuous curve is generated by performing a bubble pressure calculation at various points while varying the mole fraction from 0.0 to 1.0. The temperature remains constant. The plot is created using the excess enthalpy for the first liquid phase.

**Figure 5.24**

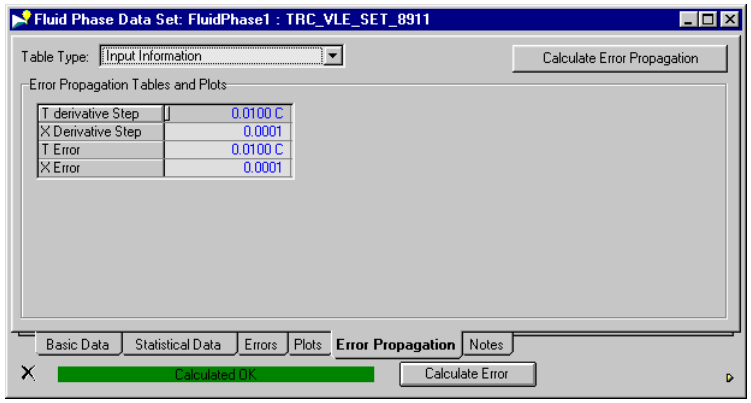



Excess Enthalpy Data Set (Benzene/Ethanol)

# 5.3.5 Error Propagation Tab

The Error Propagation tab displays the error propagation table or plots, depending on what is selected in the Table Type drop-down list in the Error Propagation tab.

**Figure 5.25**




When the Input Information option is selected in the Table Type drop-down list, the Error Propagation Tables and Plots group contains a table as shown in the figure above.

The Input Information table allows you to specify the following variables used to calculate the error propagation:

- T Derivative Step
- X Derivative Step
- T Error
- X Error

**The error propagation tables and plots will appear blank until you click the Calculate Error Propagation button.**

# Error Propagation Tables

The following sections describe the error propagation tables.

## Bubble Pressures and Compositions

The following table appears only when you select Bubble Pressures and Compositions from the Table Type drop-down list in the Error Propagation tab.

**Figure 5.26**

| Number | P | Y- Acetone | Y- Methanol | Y- M-E-Ketone |
|---|---|---|---|---|
| 1.000 | 1.012 | 0.0000 | 0.1961 | 0.8039 |
| 2.000 | 1.004 | 0.0000 | 0.3193 | 0.6807 |
| 3.000 | 1.006 | 0.0000 | 0.3859 | 0.6141 |
| 4.000 | 0.9976 | 0.0000 | 0.4589 | 0.5411 |
| 5.000 | 1.011 | 0.0000 | 0.5368 | 0.4632 |
| 6.000 | 1.016 | 0.0000 | 0.6324 | 0.3676 |
| 7.000 | 1.023 | 0.0000 | 0.7052 | 0.2948 |
| 8.000 | 1.019 | 0.0000 | 0.7802 | 0.2198 |
| 9.000 | 1.022 | 0.0000 | 0.8364 | 0.1636 |
| 10.00 | 1.022 | 0.0000 | 0.8454 | 0.1546 |
| 11.00 | 1.023 | 0.0000 | 0.8708 | 0.1292 |

| Column | Data Contained in Column |
|---|---|
| **Number** | Displays the data point number. |
| **P** | Displays the bubble pressure. |
| **Y-Component** | This and the remaining columns display the composition of the vapour at the bubble point for every component in the data set. |

## Absolute Errors in %

The following table appears only when you select Absolute Errors in % from the Table Type drop-down list in the Error Propagation tab.

**Figure 5.27**

| Number | P | Y- Acetone | Y- Methanol | Y- M-E-Ketone |
|---|---|---|---|---|
| 1.000 | 1.492e-003 | <empty> | 1.602 | 0.3830 |
| 2.000 | 9.167e-003 | <empty> | 3.661 | 1.629 |
| 3.000 | 7.365e-003 | <empty> | 2.355 | 1.425 |
| 4.000 | 1.539e-002 | <empty> | 1.307 | 1.082 |
| 5.000 | 2.329e-003 | <empty> | 1.676 | 1.874 |
| 6.000 | 3.194e-003 | <empty> | 1.672 | 2.751 |
| 7.000 | 9.657e-003 | <empty> | 1.471 | 3.352 |
| 8.000 | 5.550e-003 | <empty> | 0.4067 | 1.417 |
| 9.000 | 8.612e-003 | <empty> | 0.5284 | 2.617 |
| 10.00 | 9.012e-003 | <empty> | 0.4072 | 2.170 |
| 11.00 | 9.188e-003 | <empty> | 0.2104 | 1.396 |

| Column | Data Contained in Column |
|---|---|
| **Number** | Displays the data point number. |
| **P** | Displays the absolute percent error of the bubble pressure. |
| **Y-Component** | This and the remaining columns display the absolute percent error of the composition of the vapour at the bubble point for every component in the data set. |

## Pressure and Vapour Residuals

The following table appears only when you select Pressure and Vapour Residuals from the Table Type drop-down list in the Error Propagation tab.

**Figure 5.28**

| Number | P | Y- Acetone | Y- Methanol | Y- M-E-Ketone |
|---|---|---|---|---|
| 1.000 | 5.078e-003 | <empty> | 0.1101 | 1.977e-002 |
| 2.000 | <empty> | <empty> | 1.028e-002 | 1.685e-002 |
| 3.000 | <empty> | <empty> | 3.573e-002 | 5.965e-002 |
| 4.000 | <empty> | <empty> | 2.525e-002 | 1.421e-002 |
| 5.000 | <empty> | <empty> | 1.836e-002 | 1.348e-002 |
| 6.000 | <empty> | <empty> | 1.394e-002 | 1.434e-002 |
| 7.000 | <empty> | <empty> | 1.289e-002 | 1.797e-002 |
| 8.000 | <empty> | <empty> | 1.350e-002 | 2.789e-002 |
| 9.000 | <empty> | <empty> | 1.477e-002 | 4.448e-002 |
| 10.00 | <empty> | <empty> | 1.502e-002 | 4.851e-002 |
| 11.00 | <empty> | <empty> | 1.578e-002 | 6.329e-002 |

| Column | Data Contained in Column |
|---|---|
| **Number** | Displays the data point number. |
| **P** | Displays the absolute residual of the bubble pressure. See **Equation (5.1)**. |
| **Y-Component** | This and the remaining columns display the absolute residual of the composition of the vapour at the bubble point for every component in the data set. See **Equation (5.2)**. |

Residuals for the bubble pressure and composition:

$$\Delta P = \frac{100\left(\left|\frac{\partial P}{\partial T}\right|\sigma_T + \sum_{i=1}^{nc}\left|\frac{\partial P}{\partial x_i}\right|\sigma_x x_i\right)}{P} \qquad (5.1)$$

$$\Delta y_i = \frac{100\left(\left|\frac{\partial y_i}{\partial T}\right|\sigma_T + \sum_{i=1}^{nc}\left|\frac{\partial y_i}{\partial x_i}\right|\sigma_x x_i\right)}{y_i} \quad (5.2)$$

*where:*

$\sigma_T$ = *error in temperature*

$\sigma_x$ = *error in molar composition*

## Vapour Derivative with Respect to Temperature

The following table appears only when you select Vapour Derivitive from the Table Type drop-down list in the Error Propagation tab

**Figure 5.29**

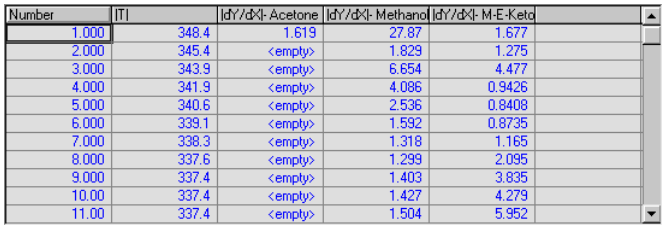
| Number | \|T\| | \|dY/dT\|- Acetone | \|dY/dT\|- Methanol | \|dY/dT\|- M-E-Keto |
|---|---|---|---|---|
| 1.000 | 348.4 | <empty> | 4.000e-004 | 4.000e-004 |
| 2.000 | 345.4 | <empty> | 5.928e-004 | 5.928e-004 |
| 3.000 | 343.9 | <empty> | 6.785e-004 | 6.785e-004 |
| 4.000 | 341.9 | <empty> | 7.597e-004 | 7.597e-004 |
| 5.000 | 340.6 | <empty> | 8.285e-004 | 8.285e-004 |
| 6.000 | 339.1 | <empty> | 8.863e-004 | 8.863e-004 |
| 7.000 | 338.3 | <empty> | 8.923e-004 | 8.923e-004 |
| 8.000 | 337.6 | <empty> | 8.318e-004 | 8.318e-004 |
| 9.000 | 337.4 | <empty> | 7.191e-004 | 7.191e-004 |
| 10.00 | 337.4 | <empty> | 6.949e-004 | 6.949e-004 |
| 11.00 | 337.4 | <empty> | 6.174e-004 | 6.174e-004 |

| Column | Data Contained in Column |
|---|---|
| **Number** | Displays the data point number. |
| **\|T\|** | Displays the bubble temperature. |
| **\|dY/dT\|-Component** | The remaining columns display the derivative of the vapour composition with respect to the bubble temperature for every component in the data set. |

## Vapour Derivative with Respect to Liquid Composition

The following table appears only when you select Vapour Derivitive in X from the Table Type drop-down list in the Error Propagation tab.

**Figure 5.30**



| Number | \|T\| | \|dY/dX\|- Acetone | \|dY/dX\|- Methanol | \|dY/dX\|- M-E-Keto |
|---|---|---|---|---|
| 1.000 | 348.4 | 1.619 | 27.87 | 1.677 |
| 2.000 | 345.4 | <empty> | 1.829 | 1.275 |
| 3.000 | 343.9 | <empty> | 6.654 | 4.477 |
| 4.000 | 341.9 | <empty> | 4.086 | 0.9426 |
| 5.000 | 340.6 | <empty> | 2.536 | 0.8408 |
| 6.000 | 339.1 | <empty> | 1.592 | 0.8735 |
| 7.000 | 338.3 | <empty> | 1.318 | 1.165 |
| 8.000 | 337.6 | <empty> | 1.299 | 2.095 |
| 9.000 | 337.4 | <empty> | 1.403 | 3.835 |
| 10.00 | 337.4 | <empty> | 1.427 | 4.279 |
| 11.00 | 337.4 | <empty> | 1.504 | 5.952 |

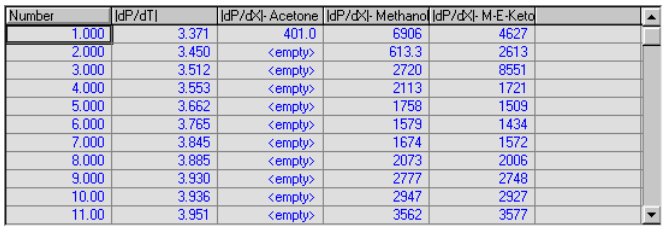
| Column | Data Contained |
|---|---|
| **Number** | Displays the data point number. |
| **\|T\|** | Displays the bubble temperature. |
| **\|dY/dX\|-** ***Component*** | The remaining columns display the derivative of the vapour composition with respect to the liquid composition of every component in the data set. |

No cross derivatives are calculated.

## Pressure Derivative with Respect to Temperature and Liquid Composition

The following table appears only when you select Pressure Derivitive in T and X from the Table Type drop-down list in the Error Propagation tab.

**Figure 5.31**



| Number | \|dP/dT\| | \|dP/dX\|- Acetone | \|dP/dX\|- Methanol | \|dP/dX\|- M-E-Keto |
|---|---|---|---|---|
| 1.000 | 3.371 | 401.0 | 6906 | 4627 |
| 2.000 | 3.450 | <empty> | 613.3 | 2613 |
| 3.000 | 3.512 | <empty> | 2720 | 8551 |
| 4.000 | 3.553 | <empty> | 2113 | 1721 |
| 5.000 | 3.662 | <empty> | 1758 | 1509 |
| 6.000 | 3.765 | <empty> | 1579 | 1434 |
| 7.000 | 3.845 | <empty> | 1674 | 1572 |
| 8.000 | 3.885 | <empty> | 2073 | 2006 |
| 9.000 | 3.930 | <empty> | 2777 | 2748 |
| 10.00 | 3.936 | <empty> | 2947 | 2927 |
| 11.00 | 3.951 | <empty> | 3562 | 3577 |

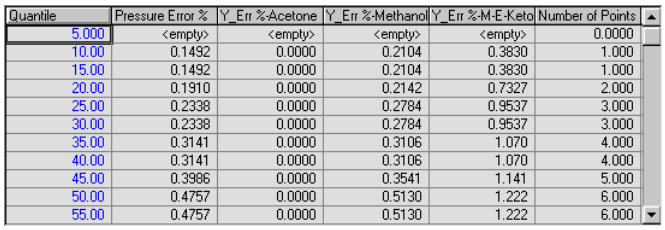
| Column | Data Contained in Column |
|---|---|
| **Number** | Displays the data point number. |

| Column | Data Contained in Column |
|---|---|
| **\|dP/dT\|** | Displays the derivative of the bubble pressure with respect to temperature. |
| **\|dP/dX\|-Component** | The remaining columns display the derivative of the pressure with respect to the liquid composition for every component in the data set. |

## Table of Quantiles

The following table appears only when you select Table of Quantiles from the Table Type drop-down list in the Error Propagation tab.

**Figure 5.32**



| Quantile | Pressure Error % | Y_Err %-Acetone | Y_Err %-Methanol | Y_Err %-M-E-Keto | Number of Points |
|---|---|---|---|---|---|
| 5.000 | <empty> | <empty> | <empty> | <empty> | 0.0000 |
| 10.00 | 0.1492 | 0.0000 | 0.2104 | 0.3830 | 1.000 |
| 15.00 | 0.1492 | 0.0000 | 0.2104 | 0.3830 | 1.000 |
| 20.00 | 0.1910 | 0.0000 | 0.2142 | 0.7327 | 2.000 |
| 25.00 | 0.2338 | 0.0000 | 0.2784 | 0.9537 | 3.000 |
| 30.00 | 0.2338 | 0.0000 | 0.2784 | 0.9537 | 3.000 |
| 35.00 | 0.3141 | 0.0000 | 0.3106 | 1.070 | 4.000 |
| 40.00 | 0.3141 | 0.0000 | 0.3106 | 1.070 | 4.000 |
| 45.00 | 0.3986 | 0.0000 | 0.3541 | 1.141 | 5.000 |
| 50.00 | 0.4757 | 0.0000 | 0.5130 | 1.222 | 6.000 |
| 55.00 | 0.4757 | 0.0000 | 0.5130 | 1.222 | 6.000 |

You can change these to any number you want; recalculate the Table of Quantiles by clicking the **Calculate Error Propagation** button.

| Column | Data Contained in Column |
|---|---|
| **Quantile** | Displays the quantiles, with the defaults as shown. |
| **Pressure Error %** | Displays the percent error in pressure. |
| **Y_Err %-Component (remaining columns except for last)** | Displays the percent error in vapour composition of all components in the data set. |
| **Number of Points (last column)** | Displays the number of points belonging to that quantile. |

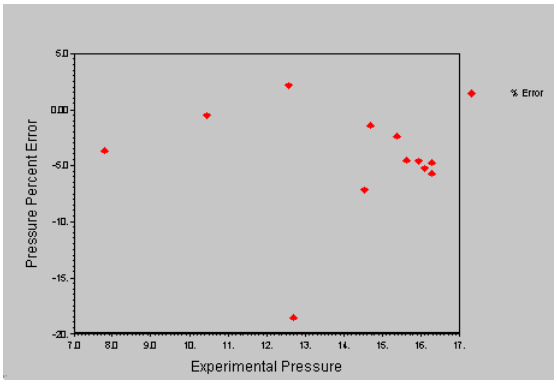
# Error Propagation Plots

The following sections describe the error propagation plots.

## Pressure Error Plot

The Pressure Error plot displays the Pressure Percent Error vs. Experimental Pressure for each data point.

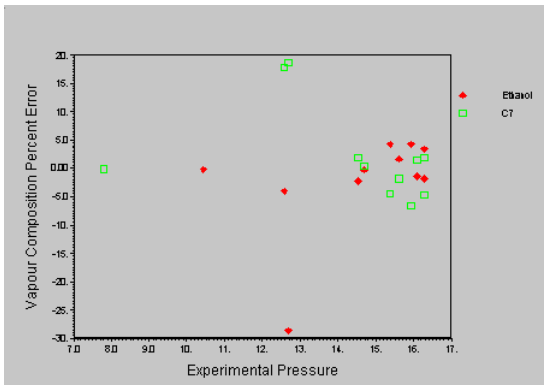
**Figure 5.33**



### Vapour Composition Error Plot

The Vapour Composition Error Plot displays the Vapour Composition Percent Error (for all components) vs. the Experimental Pressure.

**Figure 5.34**




## 5.3.6 Notes Tab

The Notes tab allows you to:

- Change the name of the FPDS view by entering a new name in the **Name** field.
- Enter information regarding the active data set in the **Notes** text editor.

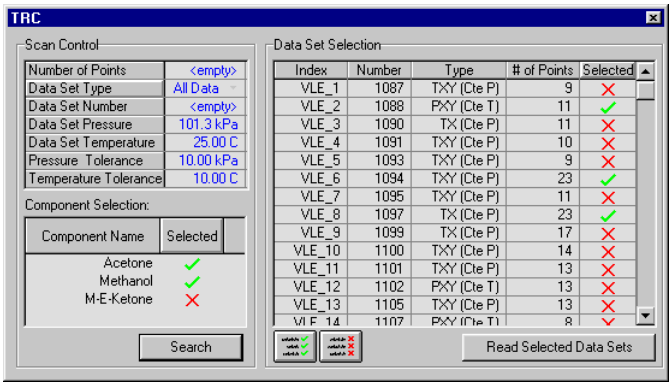
Any changes made to the information in the Notes text editor also appear in the Data Set Notes text editor of the Fluid Phase Regression view, Summary tab.

# 5.4 TRC View

To access the TRC view, refer to the **Importing Data from TRC Database** section.

The TRC view allows you to search for data sets.

**Figure 5.35**




The following table lists and describes the filter search options available in the TRC view:

To find all data set types, select the All Data option from the drop-down list.

| Object | Icon | Description |
|---|---|---|
| **Number of Points cell** | | Allows you to filter the list of possible data sets to include only data sets with a minimum number of experimental data points. |
| **Data Set Type drop-down list** | | Allows you to filter the list of possible data sets to include only certain data set types. |
| **Data Set Number cell** | | Allows you to filter the list of possible data sets to include only the data set with the same designated number as the number entered in the cell. |
| **Data Set Pressure cell** | | Allows you to filter the list of possible data sets to include only the data set generated at the specified pressure. |
| **Data Set Temperature cell** | | Allows you to filter the list of possible data sets to include only the data set generated at the specified temperature. |
| **Pressure Tolerance cell** | | Allows you to expand or contract the range of pressures in the filter search. |
| **Temperature Tolerance cell** | | Allows you to expand or contract the range of temperatures in the filter search. |

The default setting in the table is that all components in the fluid package are selected.

| Object | Icon | Description |
|---|---|---|
| **Component Selection table** |   | Allows you to select the two components for the data set you want.<br>• A green checkmark indicates that the component or data set is selected.<br>• A red cross indicates that the component or data set is not selected. |
| **Search button** | | Allows you to search for data sets based on the filter options in the Scan Control group.<br>If you change any of the filter options in the Scan Control group, click this button again to update the list of data sets to match the new filter options. |
| **Data Set Selection table** | | Displays the list of data sets found based on the filter options in the Scan Control group. |
| **Select All Data Sets icon** |  | Allows you to select all the data sets in the Data Set Selection table. |
| **Unselect All Data Sets icon** |  | Allows you to deselect all the data sets in the Data Set Selection table. |
| **Read Selected Data Sets button** | | Allows you to import the selected data sets in the Data Set Selection table into the Fluid Phase Regression view. |

# 6 Stream Manager

# 6.1 Introduction

The Stream Manager operation allows you to define any number of streams and display them in a Worksheet format similar to the Workbook in the HYSYS line of products. You can use the Stream Manager operation to compare how different property packages and properties affect the prediction of stream properties.

The Stream operation lets you define certain stream conditions and examine the properties of individual streams. The program automatically performs flash calculations on streams if the degrees of freedom for the system is satisfied (i.e., it contains the variables required to fully specify a stream). You can also examine the pressure-temperature relationship for any stream of known composition in the Stream operation, including streams with only one component.

## 6.1.1 Flash Calculations

In order for a stream to 'flash', the following information must be specified:

- Stream Composition

Two of the following properties must also be specified. At least one of the specifications must be temperature or pressure.

- Temperature
- Pressure
- Vapour Fraction
- Enthalpy

If you specify a vapour fraction of 0 or 1, the stream is assumed to be at the bubble point or dew point, respectively.

Depending on which of the state variables are known, the correct flash calculation will automatically be performed, unless you have changed the Flash Type. Once a stream is flashed, provided a flow is known, all other properties about the stream are known as well.

The following table list the different flash types available in the program:

| Flash Type | Description |
|---|---|
| **Determined Internally** | This is the default and is generally the best choice. The software will make the appropriate flash type selection. |
| **Temperature-Pressure** | You must specify the temperature and pressure in the stream in order for it to flash. If you specified a vapour fraction, it will be overwritten. |
| **Pressure-Vapour Fraction** | You must specify the pressure and vapour fraction in the stream in order for it to flash. If you specified a temperature, it will be overwritten. |
| **Temperature-Vapour Fraction** | You must specify the temperature and vapour fraction in the stream in order for it to flash. If you specified a pressure, it will be overwritten. |
| **Bubble Temperature** | You must specify the temperature in the stream in order for it to flash. A vapour fraction of 0 is automatically assigned to the stream. |
| **Bubble Pressure** | You must specify the pressure in the stream in order for it to flash. A vapour fraction of 0 is automatically assigned to the stream. |
| **Dew Temperature** | You must specify the temperature in the stream in order for it to flash. A vapour fraction of 1 is automatically assigned to the stream. |
| **Dew Pressure** | You must specify the pressure in the stream in order for it to flash. A vapour fraction of 1 is automatically assigned to the stream. |

For more information regarding the Flash calculation, refer to **Chapter 6 - Flash Calculations** in the **COMThermo Reference Guide**.

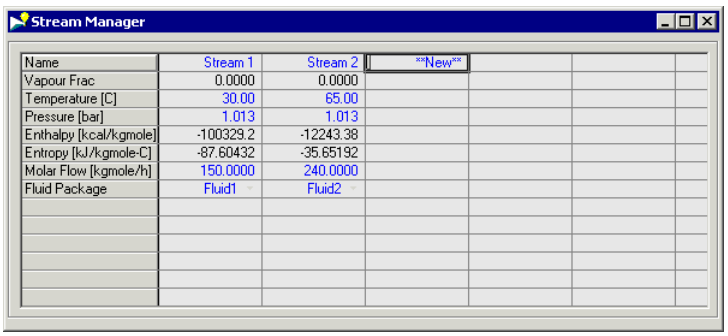
# 6.2 Stream Manager View

To access the Stream Manager view, do one of the following:

- Click on the **Stream Manager** icon in the tool bar.
- From the **Managers** menu, select **Streams Manager**.

Stream Manager icon

**Figure 6.1**




The Stream Manager view is the parent view of the Stream view.

The Stream Manager view allows you to generate streams and define some of the property values, such as fluid package, vapour fraction, temperature, pressure, enthalpy, and molar flow rate.

For more information on Stream view, refer to **Section 6.3 - Stream View**.

Access the Stream view of the individual stream to define other properties such as mass flow rate, liquid volume flow rate, and flash calculation.

## 6.2.1 Adding a Stream

To add a stream:

1. Open the Stream Manager view.
2. Click on the Name cell containing **New**.
3. Enter a name for the stream, and press the ENTER key.
4. In the other cells, define values for the properties.
   You can define any of the properties shown in the view except for **Entropy**.
5. Double-click on any of the cells (except **Fluid Package** and **Molar Flow**) in the appropriate stream column to open the Stream view.
6. Enter the rest of the required information in the Stream view.
7. To return to the Stream Manager view, click the **Close** icon on the Stream view.

The number of property values that you can define depends on the available degrees of freedom.

The program will automatically calculate the missing values for all properties when all of the basic information has been specified.

## 6.2.2 Specifying the Fluid Package

To select a fluid package for a stream:

1. Open the Stream Manager view.
2. In the **Fluid Package** cell, click the down arrow to open a drop-down list.
3. From the drop-down list, select the required fluid package.

You can access the Fluid Package view to edit the fluid package by double-clicking in the Fluid Package cell.

## 6.2.3 Specifying Composition

To specify the composition of a stream:

1. Open the Stream Manager view.
2. Double-click on the **Molar Flow** cell of the selected stream.
   The Input Composition for Stream view appears.
3. Enter the composition fraction for the current stream and click the **OK** button.

Refer to **Section 6.3.2 - Composition Tab**, for more information about the Input Composition for Stream view.

## 6.2.4 Editing a Stream

To edit a stream:

1. Open the Stream Manager view.
2. in the Stream Manager table, edit the properties of the stream as required.
3. Double-click on any of the cells (except **Fluid Package** and **Molar Flow**) in the selected stream column to open the Stream view for the selected stream.

The program will automatically calculate missing values for all properties when all basic information has been specified.

4. In the Stream view, edit the other properties of the stream as required.
5. To return to the Stream Manager view, click the **Close** icon on the Stream view.

## 6.2.5 Deleting a Stream

To delete a stream:

1. Open the Stream Manager view.
2. In the **Name** cell, select the name of the stream you want to delete.
3. Press the DELETE key.

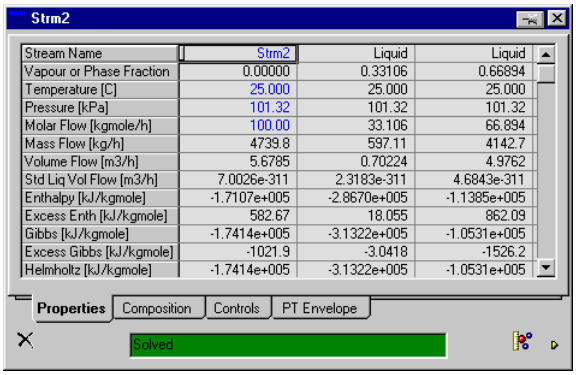
# 6.3 Stream View

Stream Manager icon

The Stream view can be accessed by doing the following:

1. Open the Stream Manager view.
2. Double-click on any of the cells (except **Fluid Package** and **Molar Flow**) under the Stream Name column for the required stream.

**Figure 6.2**




The Stream view contains four tabs: Properties, Composition, Controls, and PT Envelope. The view also contains four objects at the bottom of the view. The following table lists and describes the objects available in the Stream view:

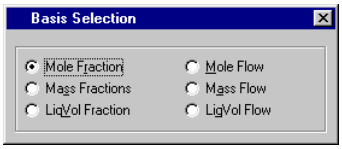
| Object | Icon | Description |
|---|---|---|
| **Delete icon** | | Allows you to delete the current stream. |
| **Status bar** | | Displays the status of the current stream. |
| **Change... Basis icon** | | Allows you to change the composition fraction basis displayed in the Composition tab of the current Stream view. |
| **Open Page Tab as Separate Window icon** | | Allows you to open the active tab as a separate view. |

For more information about the composition fraction basis, refer to the **Basis Selection View** section.

# Basis Selection View

The Basis Selection view allows you to change the composition basis fraction type displayed in the Composition tab.

**Figure 6.3**




Change Composition Fraction Basis icon

To change the composition basis using the Basis Selection view:

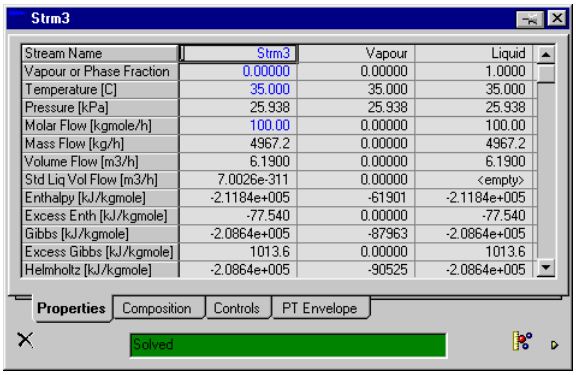
1. Click on the **Change Composition Fraction Basis** icon to open the Basis Selection view.
2. Use the radio buttons to select the composition basis you want to display in the **Composition** tab.
3. Click the **Close** icon when you are done.

The following sections describe in detail each tabs available in the Stream view.

# 6.3.1 Properties Tab

The Properties tab allows you to view and manipulate the properties of the current stream.

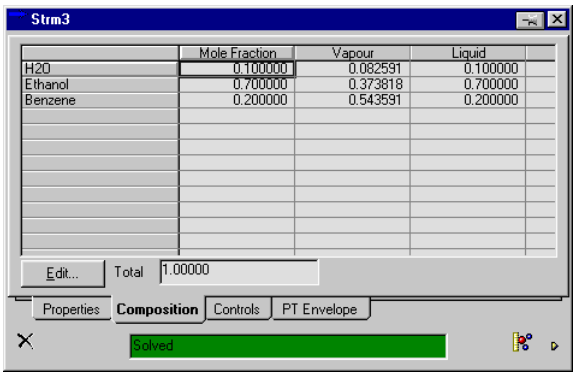
**Figure 6.4**




# 6.3.2 Composition Tab

The Composition tab allows you to view and specify the composition value of the current stream.

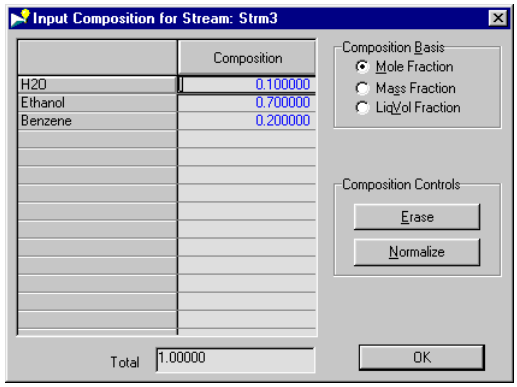
**Figure 6.5**



To specify the composition of the stream:

1. Open the Stream view.
2. Click the **Composition** tab.
3. Click the **Edit** button. The Input Composition for Stream view appears.

**Figure 6.6**




4. In the Input Composition for Stream view you can perform the following tasks:
   - Enter the stream composition fraction in the Composition cells beside the components.
   - Enter the composition values in a different composition basis type by selecting the appropriate radio button in the Composition Basis group.
   - Erase current composition values by clicking the **Erase** button.
   - Enter any value for the composition fraction, and click the **Normalize** button to ensure the total for all values equals 1.
5. When you are done, click the **OK** button. The Input Composition for Stream view automatically closes.

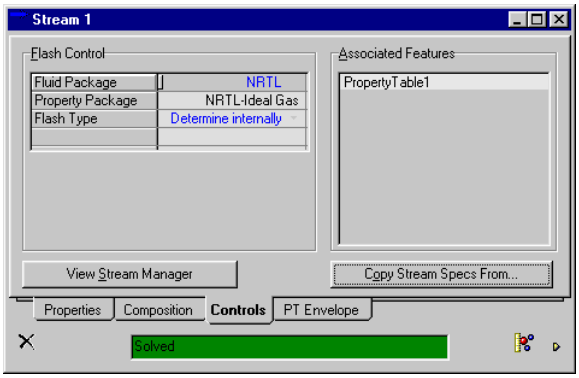
When you enter the compositions, click the Normalize button and the program ensures the total is 1.0, while also specifying any <empty> compositions as zero. If compositions are left as <empty>, the program cannot perform the flash calculation on the stream.

# 6.3.3 Controls Tab

The Controls tab allows you to manipulate the flash calculation performed on the current stream.

For more information about the flash calculation, refer to **Section 6.1.1 - Flash Calculations**.

**Figure 6.7**

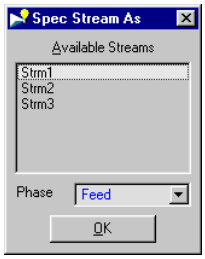



The following table lists and describes the objects in the Controls tab:

| Object | Description |
|---|---|
| **Fluid Package drop-down list** | Allows you to select a different fluid package for the current stream and flash calculation. |
| **Property Package cell** | Displays the property package associated with the selected fluid package. |
| **Flash Type drop-down list** | Allows you to select a different flash type for the flash calculation. |
| **View Stream Manager button** | Allows you to access the Stream Manager view by making the Stream Manager view a modal view. |
| **Associated features group** | Displays the operations that are using the current stream in their calculations.<br>• Double-click on the operation's name to access the operation's property view using the current stream.<br>• If there are no operations using the current stream, the list in the group will appear blank. |
| **Copy Stream Specs From button** | Allows you to access the Spec Stream As view. This view allows you to select a different stream specification and apply it to the current stream. Refer to the **Spec Stream As View** section for more information. |

For more information about modal and non-modal views, refer to **Section 2.3.4 - Modal vs. Non-Modal Views** in the **User Guide**.

## Spec Stream As View




The Spec Stream As view allows you to select the specifications of a different stream and apply the specifications to the current stream.

To apply a different specification on the stream:

1. Open the Stream Manager view.
2. Double-click on any of the cells (except **Fluid Package** and **Molar Flow**) under the Name column of the stream you want.
   The Stream view appears.
3. Click the **Controls** tab.
4. Click the **Copy Stream Specs From** button. The Spec Stream As view appears.
5. From the Available Streams list, select the stream containing the specification you want.
6. In the Phase drop-down list, select the phase type for the selected stream.
7. When you are done selecting, click the **OK** button. The Spec Stream As view automatically closes.

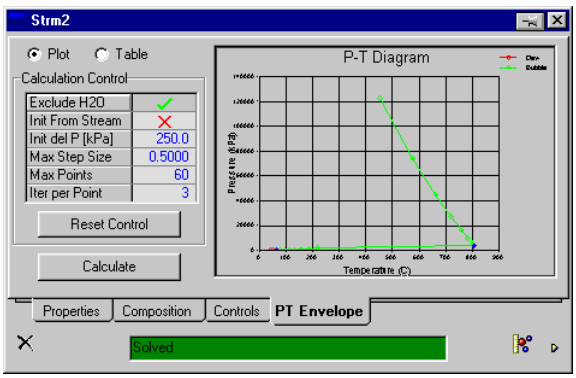
Depending on the selected stream the following phase types may be available:

- Feed
- Liquid
- Vapour

# 6.3.4 PT Envelope Tab

The PT Envelope tab allows you to manipulate the scope and accuracy of the envelope calculations in the Pressure vs. Temperature plot.

**Figure 6.8**



The following table lists and describes the objects available in the PT Envelope tab:

| Object | Description |
|---|---|
| **Plot radio button** | Allows you to examine the envelope calculation results in plot format. |
| **Table radio button** | Allows you to examine the envelope calculation results in table format. |
| **Exclude H2O checkbox** | Allows you to toggle between ignoring or including any water in the current stream as part of the calculation. |
| **Init From Stream checkbox** | Allows you to toggle between initializing or not initializing the envelope algorithm with the current stream conditions. |
| **Init del P cell** | Allows you to specify the initial change in pressure used by the algorithm. |
| **Max Step Size cell** | Allows you to control the maximum distance between points. |
| **Max Points cell** | Allows you to specify the maximum number of points to be calculated. |
| **Iter per Point cell** | Allows you to specify the number of iterations conducted on each point. |
| **Reset Control button** | Allows you to reset all the options in the Calculation Control group to the default settings. |
| **Calculate button** | Allows you to generate and display the calculated values on the plot or table. |
| **Plot** | Displays the calculated results after the Calculate button has been clicked. Available only when the Plot radio button is selected. |
| **Table** | Displays the calculated results after the Calculate button has been clicked. Available only when the Table radio button is selected. |

For low step sizes, more points will be plotted.

For high step sizes, fewer points will be plotted.

For information on manipulating plot appearance, refer to **Section 7.4 - Plot Area** and **Chapter 8 - Plot Properties** in the **User Guide**.

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# Index

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