Property Data and Models in Aspen Plus® V8.0

1. Lesson Objectives

- Learn how to retrieve properties data from NIST ThermoData Engine (aka. NIST TDE) in Aspen Plus, and compare the experimental data with the prediction by various thermodynamic models.
- Explore how to use the software to generate thermodynamic properties diagrams (e.g. T-xy, y-x).
- Perform regression analysis to increase model prediction accuracy

2. Prerequisites

- Aspen Plus V8.0
- Basic understanding of binary vapor-liquid equilibrium

3. About the NIST ThermoData Engine (TDE) in Aspen Plus

The ThermoData Engine (TDE) is a thermodynamic data correlation, evaluation, and prediction tool provided with Aspen Plus and Aspen Properties through a long-term collaboration agreement with the National Institute of Standards and Technology (NIST). The purpose of the ThermoData Engine software is to provide critically evaluated thermodynamic and transport property data based on the principles of dynamic data evaluation.

The examples presented are solely intended to illustrate specific concepts and principles. They may not reflect an industrial application or real situation.

4. Problem Statement and Aspen Plus Solution

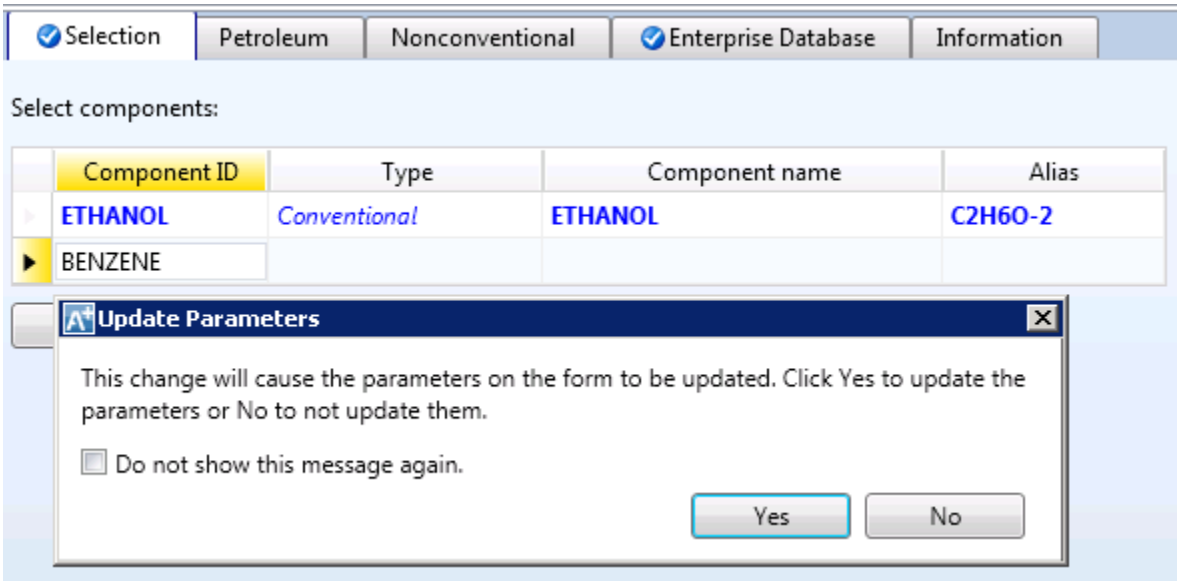
Ethanol/Benzene mixture is known to be a non-ideal binary system that exhibits azeotropic behavior in thermodynamic phase equilibrium. Using Aspen Plus, we want to compute the thermodynamic equilibrium of an Ethanol/Benzene binary mixture using different thermodynamic models, and compare the calculation results with experimental data available from the NIST ThermoData Engine.

- Citation Info of Experimental Data:
  - Ellis, S.R.M.; Thwaites, J.M., "A small-capacity equilibrium still", Chemical Processing and Engineering, v36, pp358–360, 1955
- Thermodynamic Models to Test:
  - NRTL
  - IDEAL
  - PENG-ROBINSON

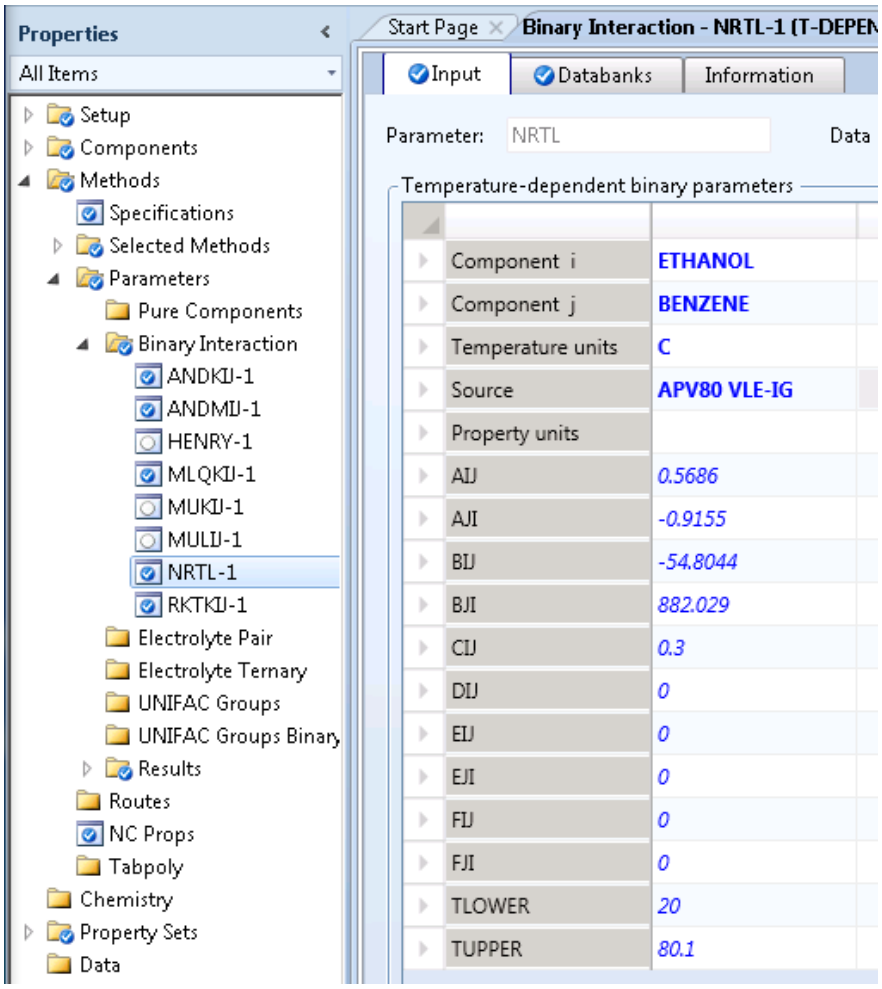
Aspen Plus Solution:

4.01. Start **Aspen Plus V8.0**. Select **New | Chemical Processes | Chemicals with Metric Units**. Click **Create**.

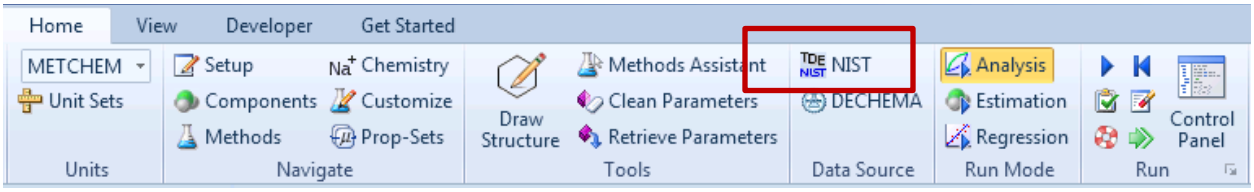
4.02. Define components. In the **Components | Specifications | Selection** tab enter **Ethanol** and **Benzene** as the **Component ID**. You will be prompted by an **Update Parameters** dialog box. Click **Yes** to update parameters.



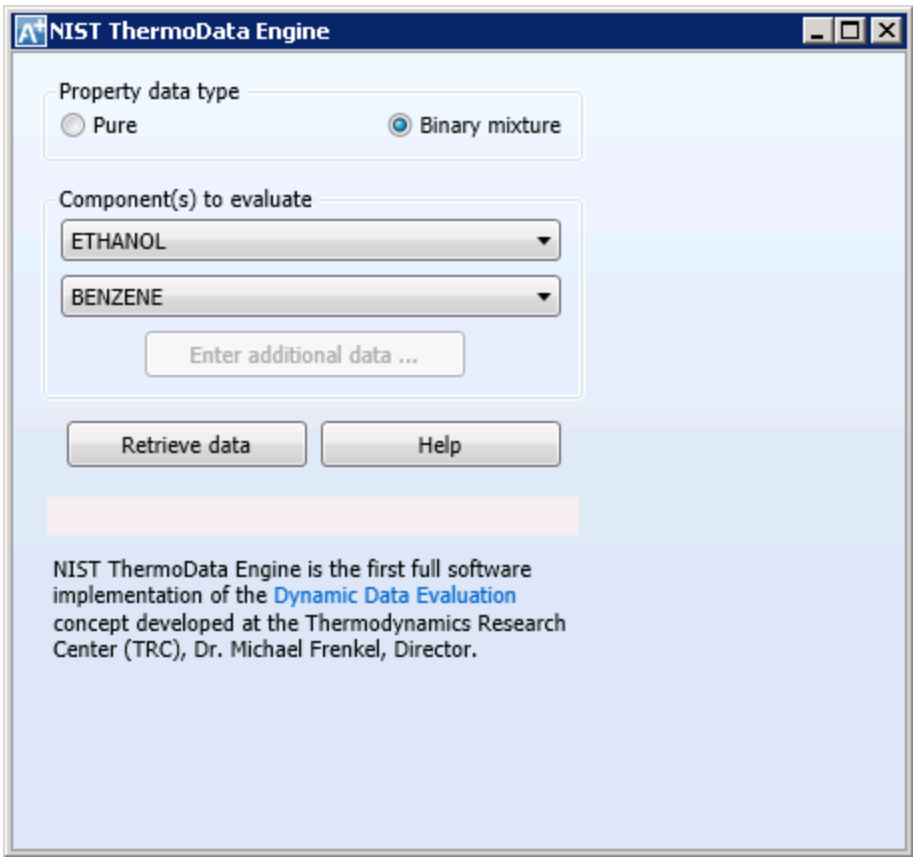
4.03. Populate the binary interaction parameters by going to **Methods | Parameters | Binary Interaction | NRTL-1**.



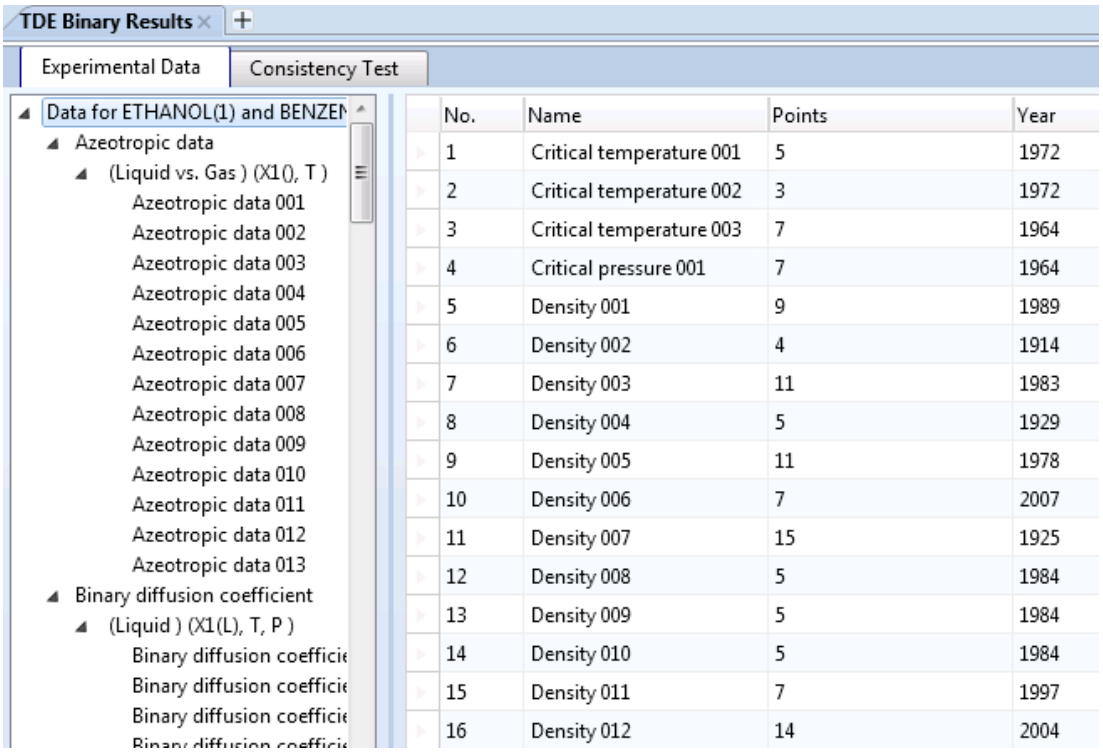
4.04. Retrieve data. Click on the **NIST** button in the home ribbon menu. It will open the **NIST ThermoData Engine** window.



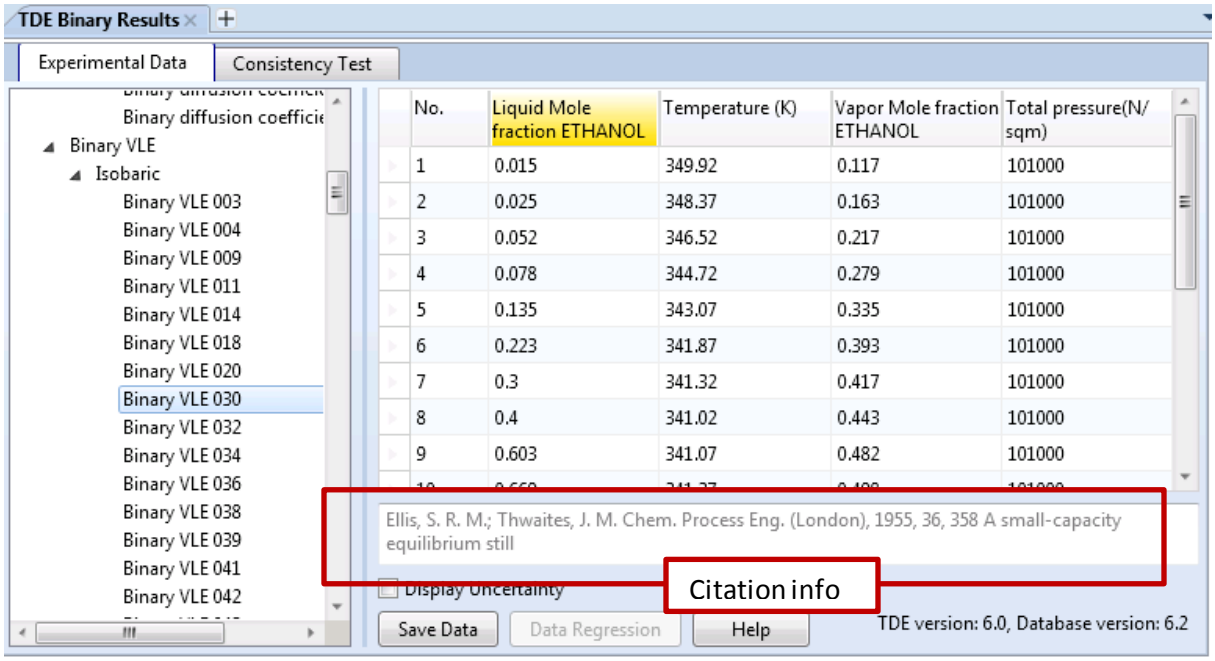
4.05. In the **NIST ThermoData Engine** window select **Binary Mixture** for **Property data type**, and **ETHANOL** and **BENZENE** for **Components**. Press the **Retrieve data** button, it will retrieve all binary data available in the NIST TDE.



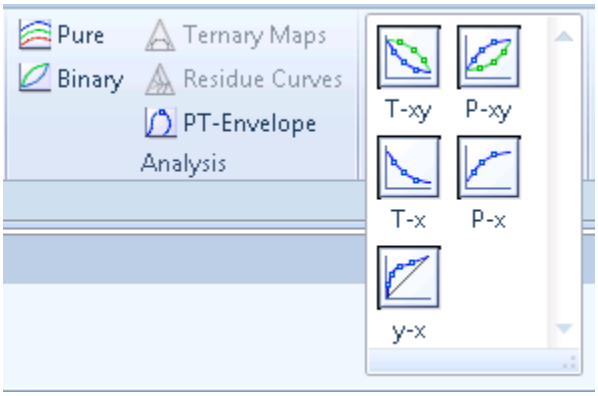
4.06. Close the **NIST ThermoData Engine** window and view the **TDE Binary Results**.

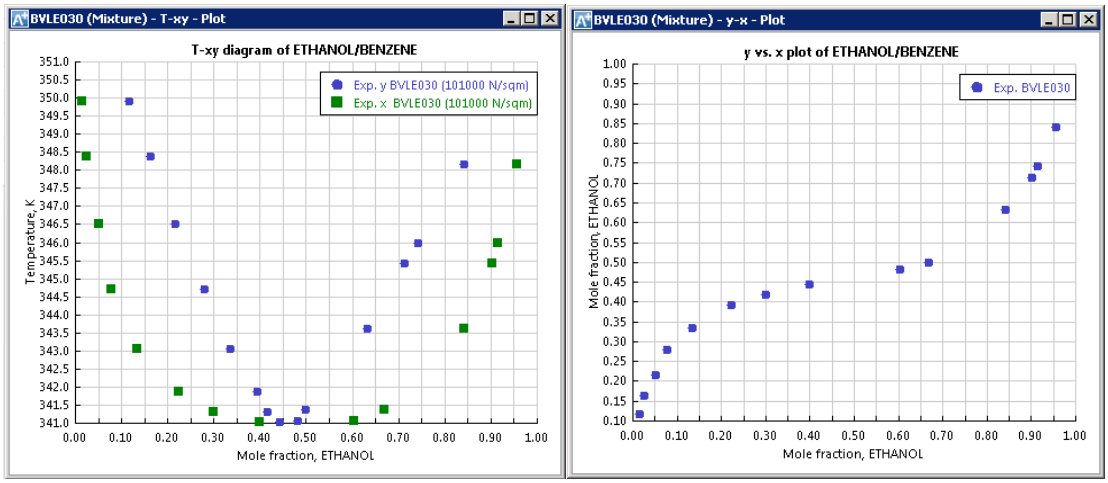


4.07. In the **TDE Binary Results**, scroll down to find the **Binary VLE | Isobaric | Binary VLE 030** data set. Select **Save Data** at the bottom of the screen, and click **OK** on the following window after confirming you have selected the correct data set. Make note of the citation information located at the bottom of the screen.



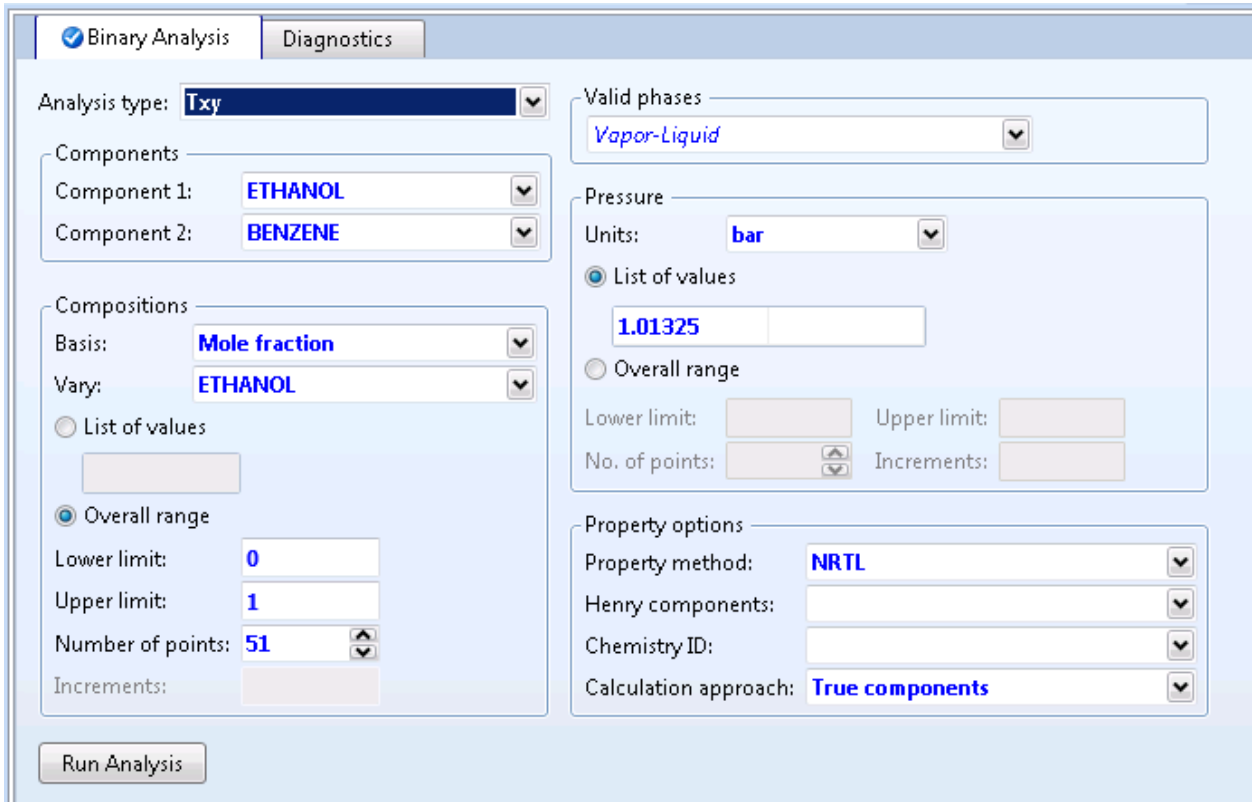
4.08. In the navigation pane go to the **Data | BVLE30 | Data** tab. Let's review the experimental data by plotting it. Since this is an Isobaric data set, you can create a T-xy equilibrium plot. Find the **Plot** buttons in the home ribbon menu. Press each **T-xy** and **y-x** plot button. You will notice this binary mixture has an azeotrope near a mole fraction of 0.45 ethanol.

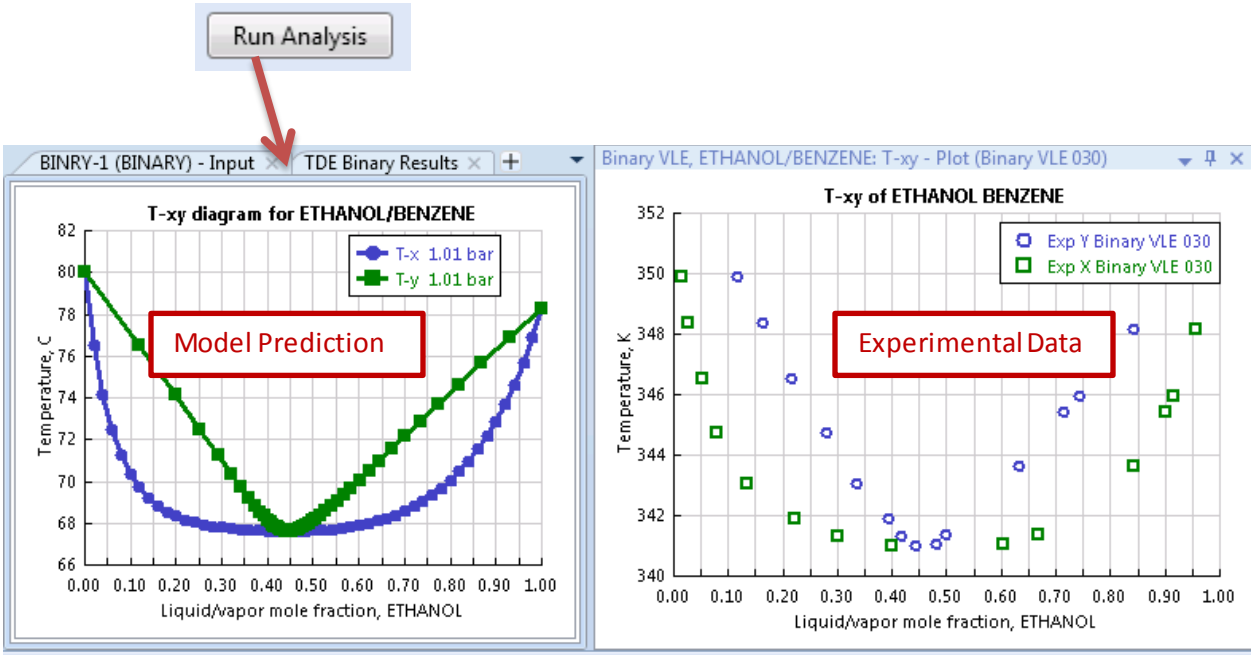




4.09. We want to test the Aspen Plus thermodynamic model by predicting these experimental data, starting with the NRTL, IDEAL, and PENG-ROBINSON base methods. Find the **Binary** icon in the **Home** ribbon menu under **Analysis**. Upon clicking, a new **Binary Analysis** window will open. Check if these settings are configured correctly then press the Run Analysis button for model predictions.

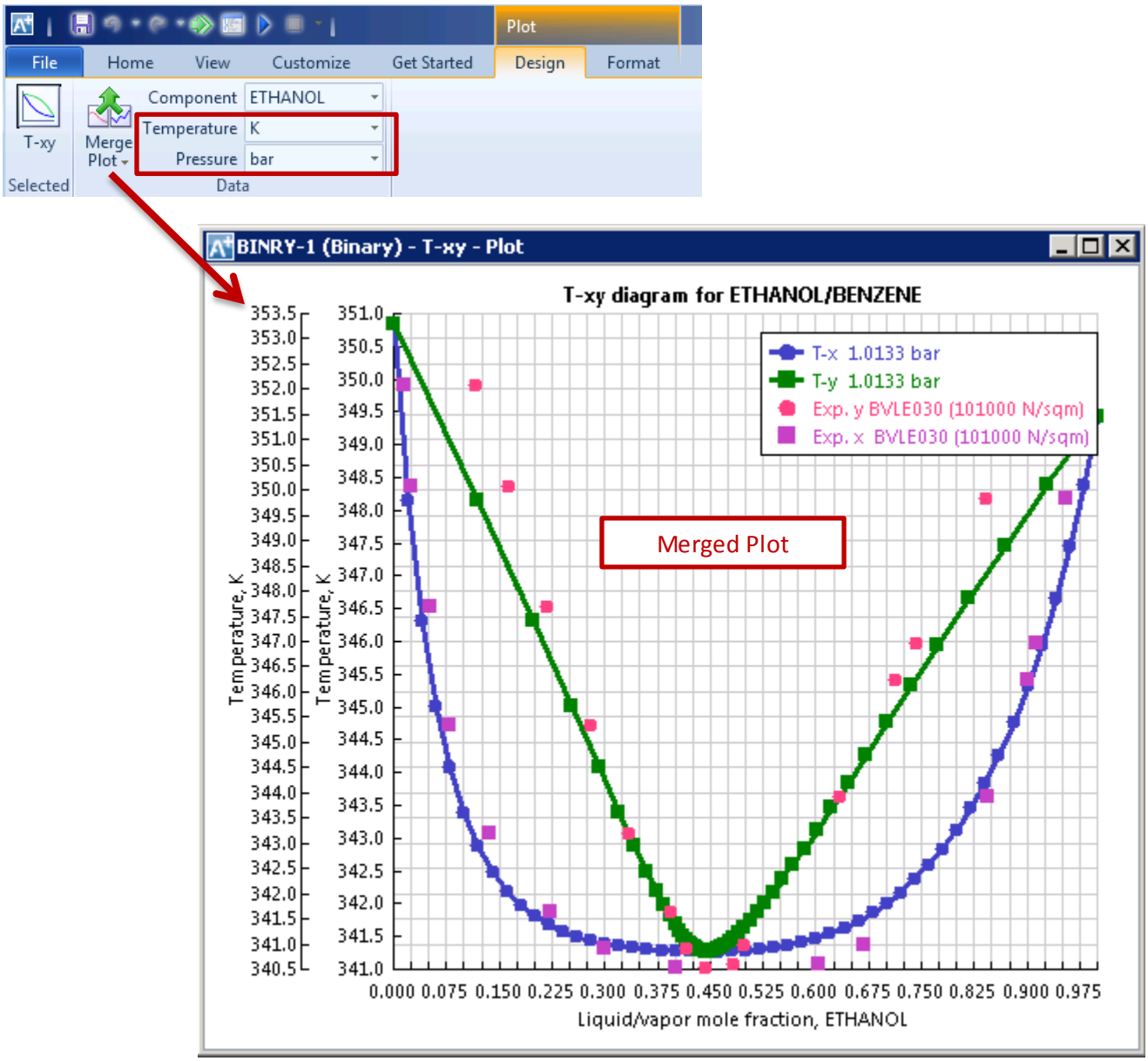
a. NRTL Model Prediction





4.10. Please note, in this example, the temperature unit in the prediction is Celsius while the experimental data unit is Kelvin. We would like to make them display the same unit (Kelvin) and merge them onto one plot so we can compare them.

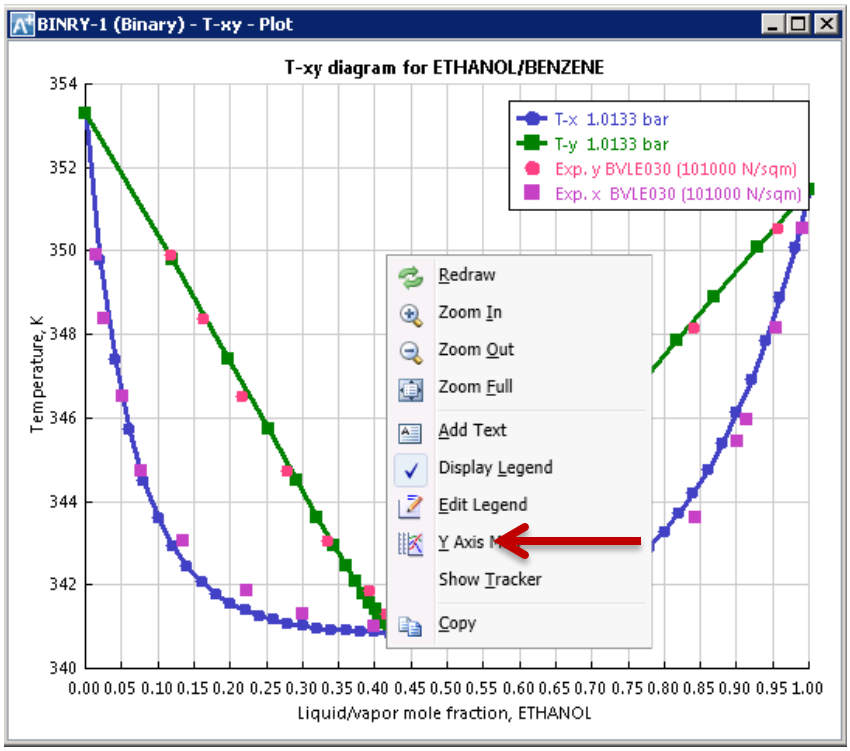
- To change the units, select the predicted Txy plot, then find the ribbon menu, **Design | Data**, and set **Temperature= K**.
- Then press the **Merge Plot** button to merge the two plots onto a single plot.



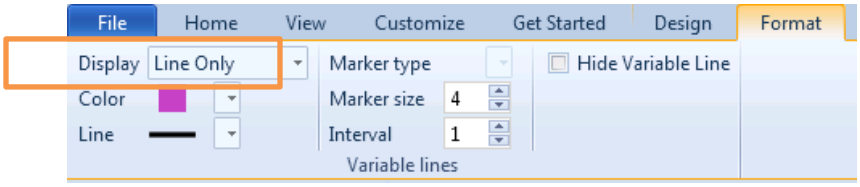
4.11. The merged plot needs some fine tuning:

- Use same Y-Axis
- Use Line only for the predicted values
- Improve legend property for clearer review

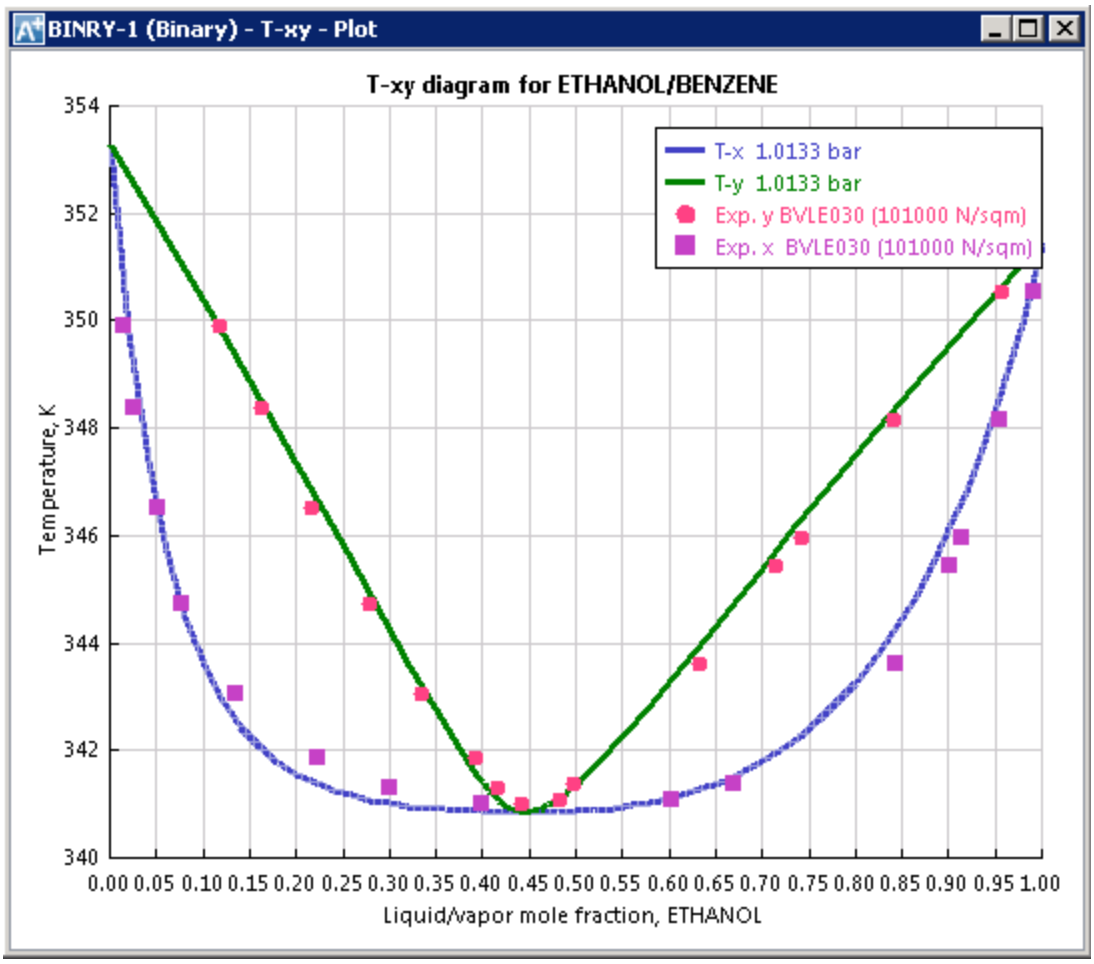
To use the same Y-Axis, right click on the plot, select **Y-Axis Map**, and press the **Single Y-Axis** button when the new window is opened. Press **OK**.



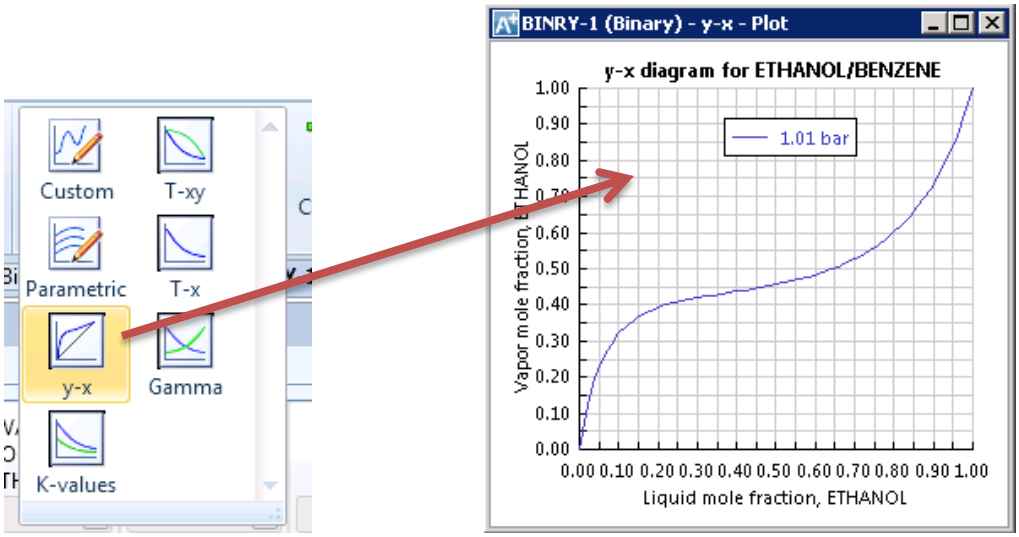
To use Line only for the predicted values, select the predicted value series on the plot, find the ribbon menu, **Format**, set **Display = Line Only**. You can change the line thickness and the color as well.



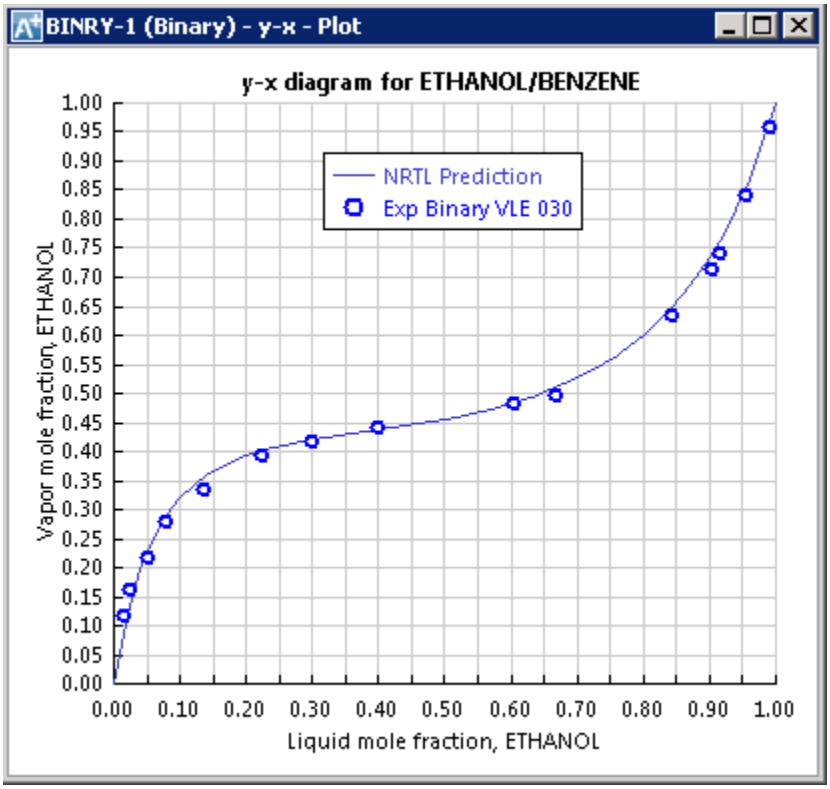
An improved T-xy plot is shown below:



4.12. To create y-x predictions, in the navigation pane go to **Analysis | BINRY-1 | Results** (which are the results of the Binary Analysis), then select the **y-x** plot button in the ribbon menu.



4.13. Similar to the T-xy plot, you can merge the predictions and experimental data into the same plot. This is shown below:



Repeat these prediction and comparison steps for **IDEAL** and **PENG-ROBINSON** models.

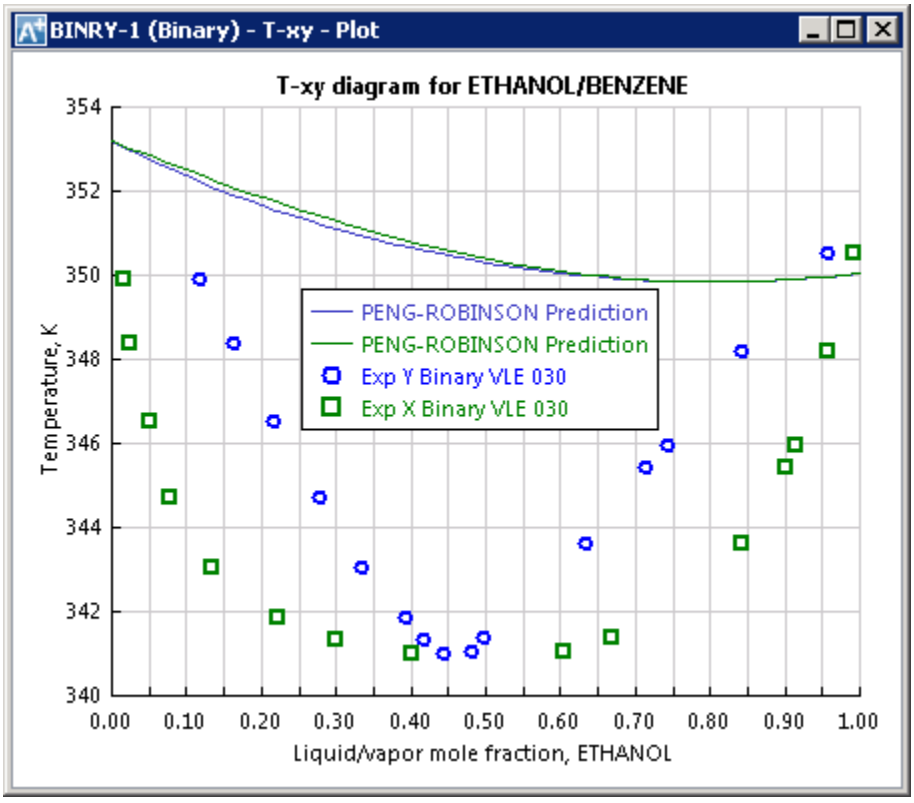
4.14. **IDEAL Model Prediction**

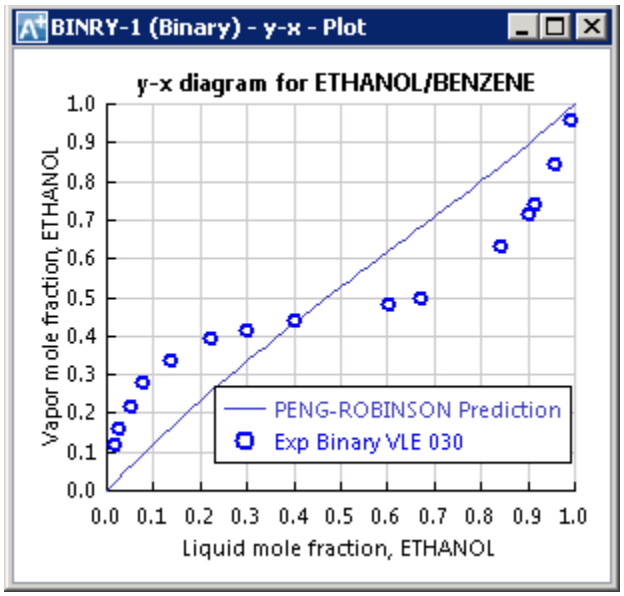
To use IDEAL method for the predictions, go to **Methods** and select **IDEAL** for **Base method**. It will add **IDEAL** to the **Selected Methods**, so that you can choose it from the **Binary Analysis** window.


Global
Flowsheet Sections
Referenced
Information
Property methods & options
Method filter: COMMON
Base method: IDEAL
Henry components:
Method name:
IDEAL
Modify
BINRY-1 (BINARY) - Input
TDE Binary Results
Methods
Binary Analysis
Diagnostics
Analysis type: Txy
Components
Component 1: ETHANOL
Component 2: BENZENE
Compositions
Basis: Mole fraction
Vary: ETHANOL
List of values
Overall range
Lower limit: 0
Upper limit: 1
Number of points: 51
Increments:
Valid phases
Vapor-Liquid
Pressure
Units: bar
List of values
1.01
Overall range
Lower limit:
No. of points:
Property options
Property method: IDEAL
Henry components:
Chemistry ID:
Calculation approach: True components
IDEAL method will be enabled in Binary Analysis
Run Analysis
IDEAL prediction compared with the experimental data.
How accurate are these predictions?
BINRY-1 (Binary) - T-xy - Plot
T-xy diagram for ETHANOL/BENZENE
IDEAL Prediction
IDEAL Prediction
Exp Y Binary VLE 030
Exp X Binary VLE 030
Liquid/vapor mole fraction, ETHANOL
Vapor mole fraction, ETHANOL
Liquid mole fraction, ETHANOL
IDEAL Prediction
Exp Binary VLE 030

b. PENG-ROBINSON Model Prediction

Similar to **IDEAL**, to use the **PENG-ROBINSON** method for the predictions, go to **Methods** and select **Base method = PENG-ROB**. It will add **PENG-ROB** to the **Selected Methods**, so that you can choose it from the **Binary Analysis** window. By using the same procedure, the following plots were created.

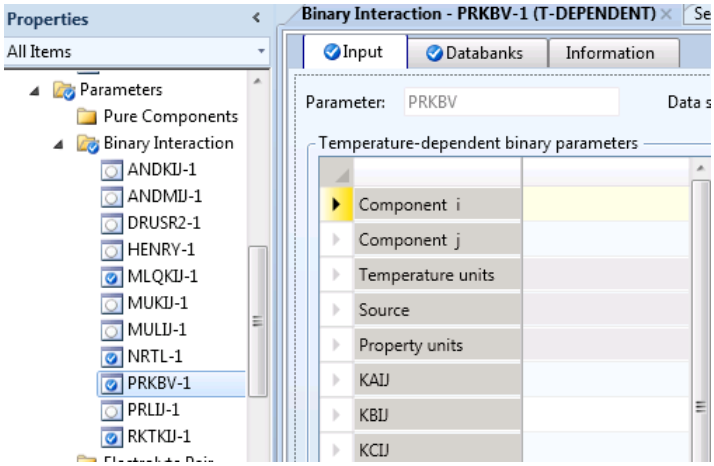




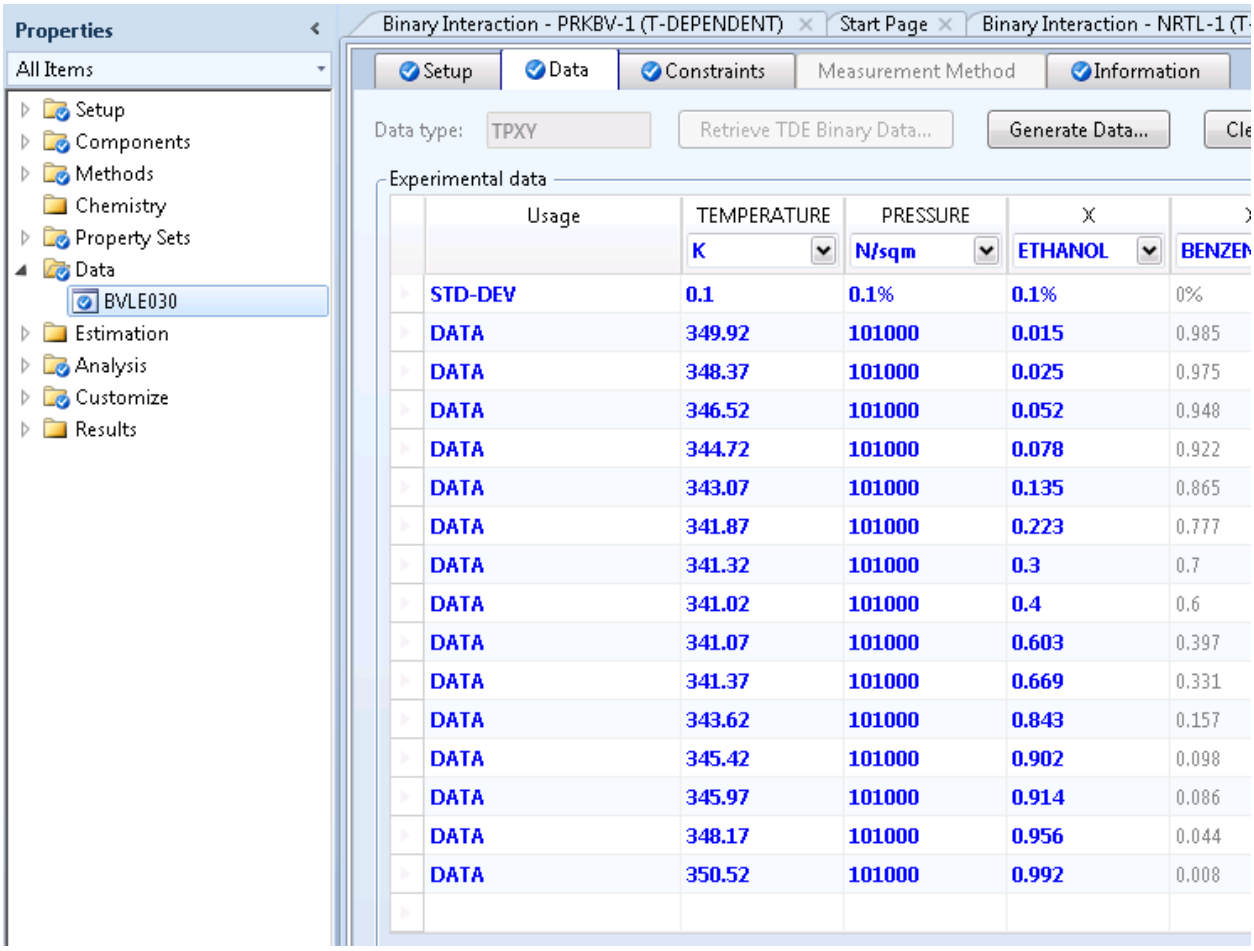
4.15. The predictions given by the Peng-Robinson method are inaccurate because Aspen Plus has not provided the binary parameters or the given binary interaction parameters are wrong. These predictions can be greatly improved by performing a regression analysis inside of Aspen Plus.

By using the regression feature, you can find 'fitted' binary interaction parameters to explain a particular binary system. Once you achieve such regression, you can extend the use of the 'fitted' thermodynamic model for process simulation. The steps to complete a regression analysis of experimental data inside Aspen Plus are listed below.

(Step 1) Go to **Methods | Parameters | Binary Interaction | PRKBV-1**, the data fields of Temperature-dependent binary parameters are all empty. This means that the PENG-ROBINSON method has no binary parameters for the ETHANOL/BENZENE mixture, therefore you cannot expect a reasonable model prediction.

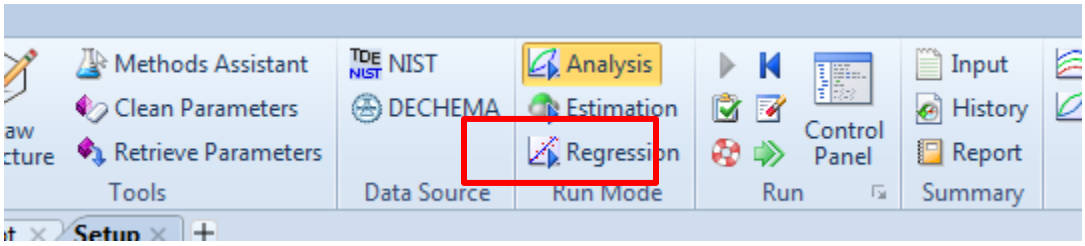


(Step 2) In order to perform a regression analysis, you need experimental data. You can get the data from **NIST TDE**. We have already retrieved this data in steps 4.04-4.07. In the navigation pane go to the **Data | BVLE030 | Data** tab to view the experimental data retrieved from NIST TDE.

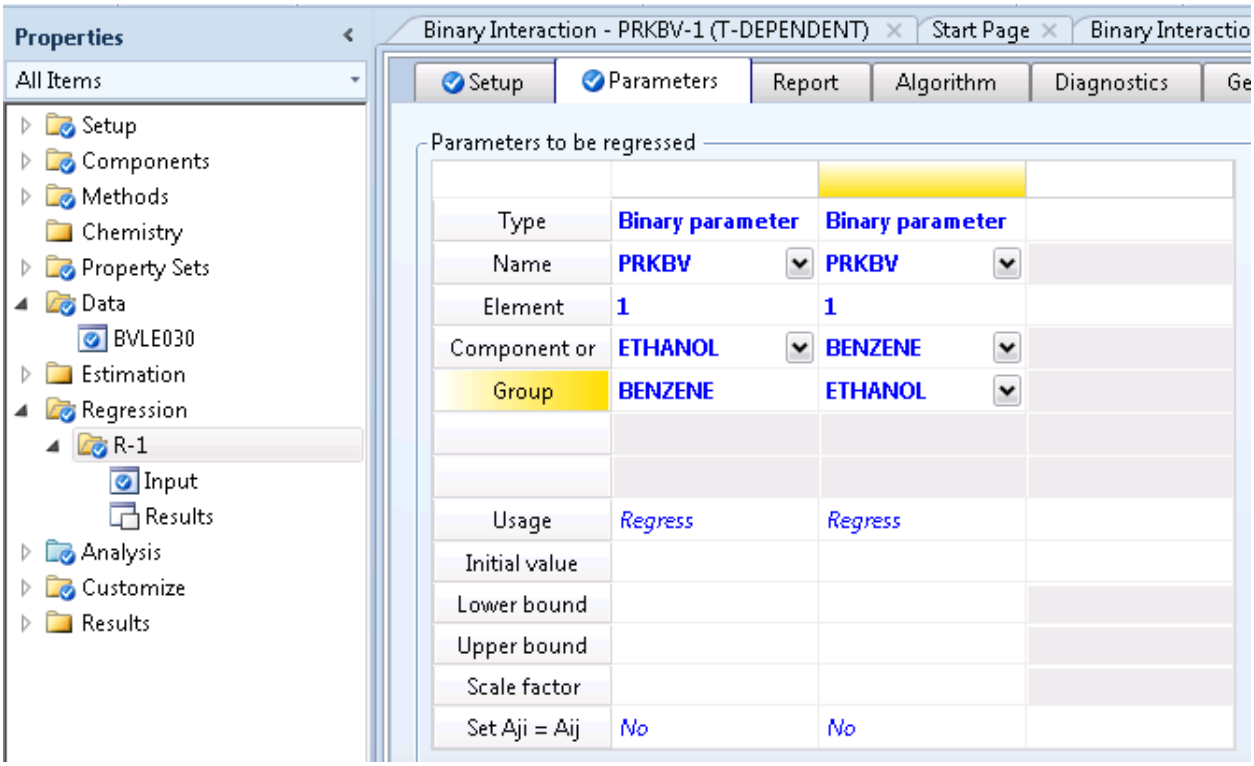


Usage	TEMPERATURE K	PRESSURE N/sqm	X ETHANOL	BENZEN
STD-DEV	0.1	0.1%	0.1%	0%
DATA	349.92	101000	0.015	0.985
DATA	348.37	101000	0.025	0.975
DATA	346.52	101000	0.052	0.948
DATA	344.72	101000	0.078	0.922
DATA	343.07	101000	0.135	0.865
DATA	341.87	101000	0.223	0.777
DATA	341.32	101000	0.3	0.7
DATA	341.02	101000	0.4	0.6
DATA	341.07	101000	0.603	0.397
DATA	341.37	101000	0.669	0.331
DATA	343.62	101000	0.843	0.157
DATA	345.42	101000	0.902	0.098
DATA	345.97	101000	0.914	0.086
DATA	348.17	101000	0.956	0.044
DATA	350.52	101000	0.992	0.008

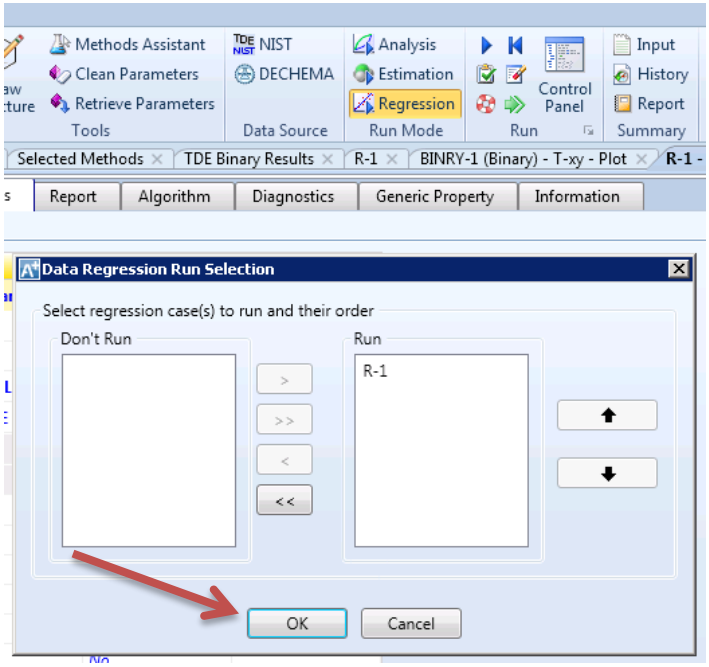
(Step 3) Create a regression. Change the run mode to **Regression**.



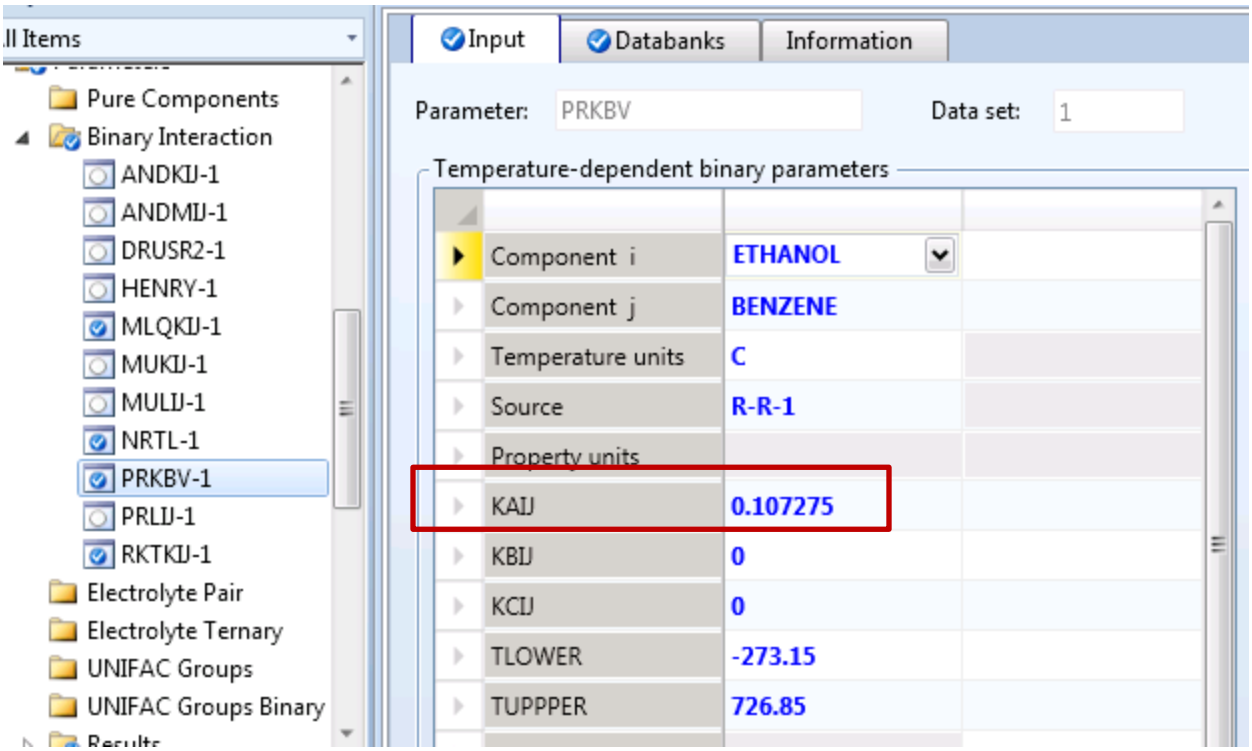
In the navigation pane go to **Regression** and press the **New** button. In the **Setup** tab select the data set to perform the regression on (**BVLE030**) and set the **Parameters** table as shown below:



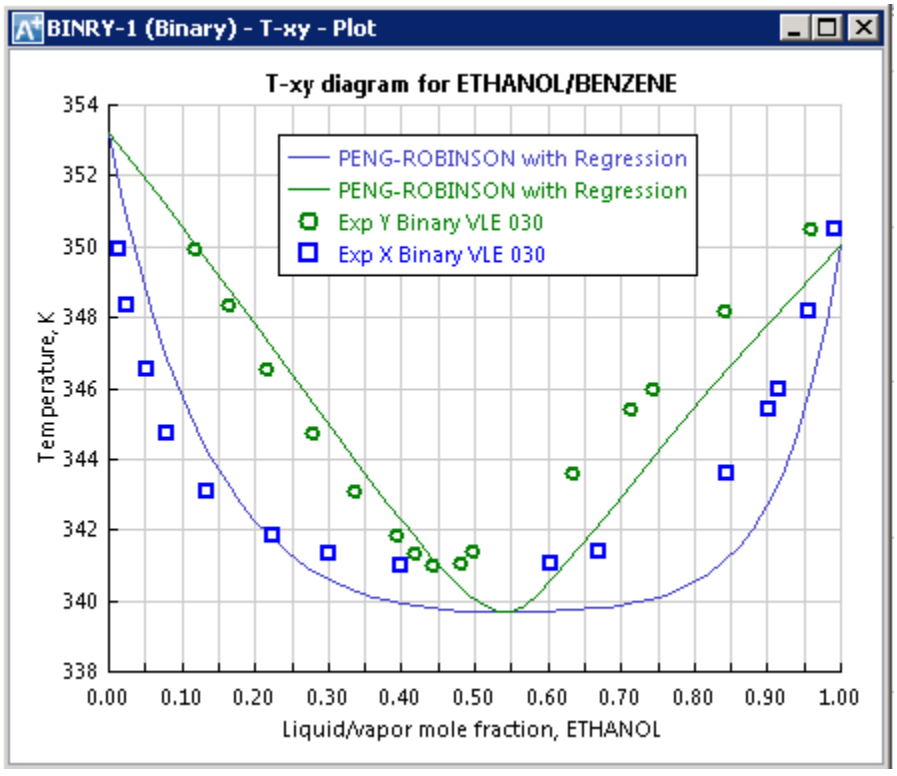
(Step 4) Run the regression (**F5**). Press **OK** when the **Data Regression Run Selection** window is shown.

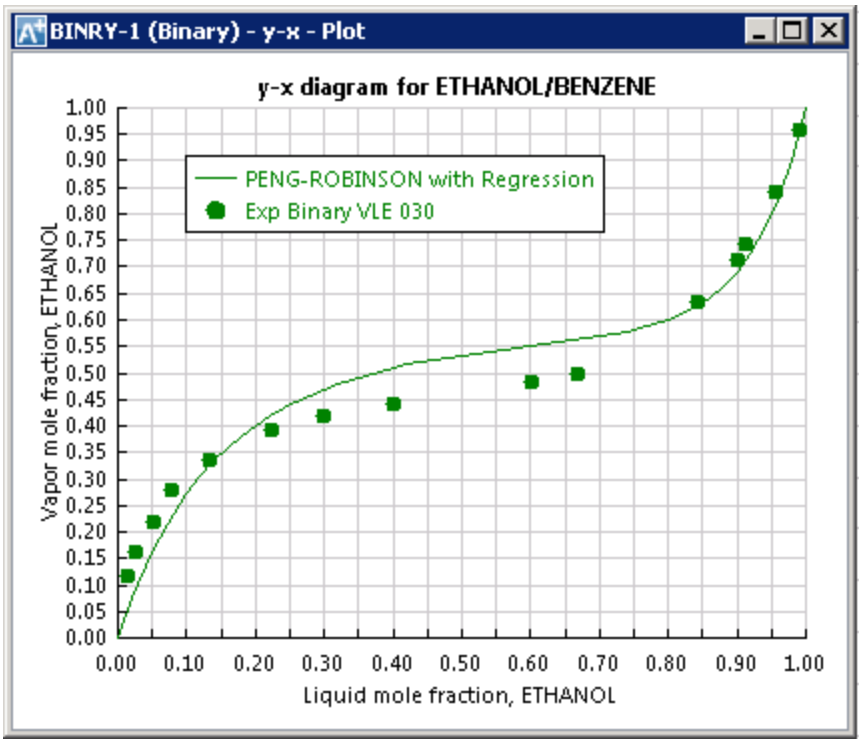


Once the regression is complete, the binary parameters data field will be filled with the 'fitted' parameters.



(Step 5) Re-predict the equilibrium by using PENG-ROBINSON with the binary parameters obtained by the regression.





You can see that the Peng-Robinson predictions are greatly improved from the original predictions. Comparing model predictions and experimental results is a good habit to develop when creating a simulation. If the model predictions are not accurate, the simulation will not provide accurate results. Regression analysis is a great tool for fine tuning model parameters and ensuring that a simulation will produce useful information about the process design.

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