

Generate Txy Diagram with Aspen Plus® V8.0

1. Lesson Objectives

- Use **Method Assistant** in Aspen Plus to determine which property method to use to create a Txy diagram for the binary system of ethane and ethylene
- Learn how to generate Txy diagrams in Aspen Plus

2. Prerequisites

- Aspen Plus V8.0

3. Background

A glance at the Txy diagram for a binary system can quickly tell whether it is easy to separate the two components. If the x-curve and y-curve are not close together and there is no azeotrope, then it is easy to separate the two components using distillation. If there is an azeotrope, then we have to use some special technologies (e.g., extractive distillation) to separate them into pure components. If the x-curve and y-curve are very close together, it is more economical to use extractive distillation to separate them into pure components. Therefore, a Txy diagram is a very useful tool for things such as process synthesis and search of solvents.

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

4. Aspen Plus Solution

If you are unfamiliar with how to start Aspen Plus, select components, or define methods, consult **Get Started Guide for New Users of Aspen Plus.pdf** for instructions.

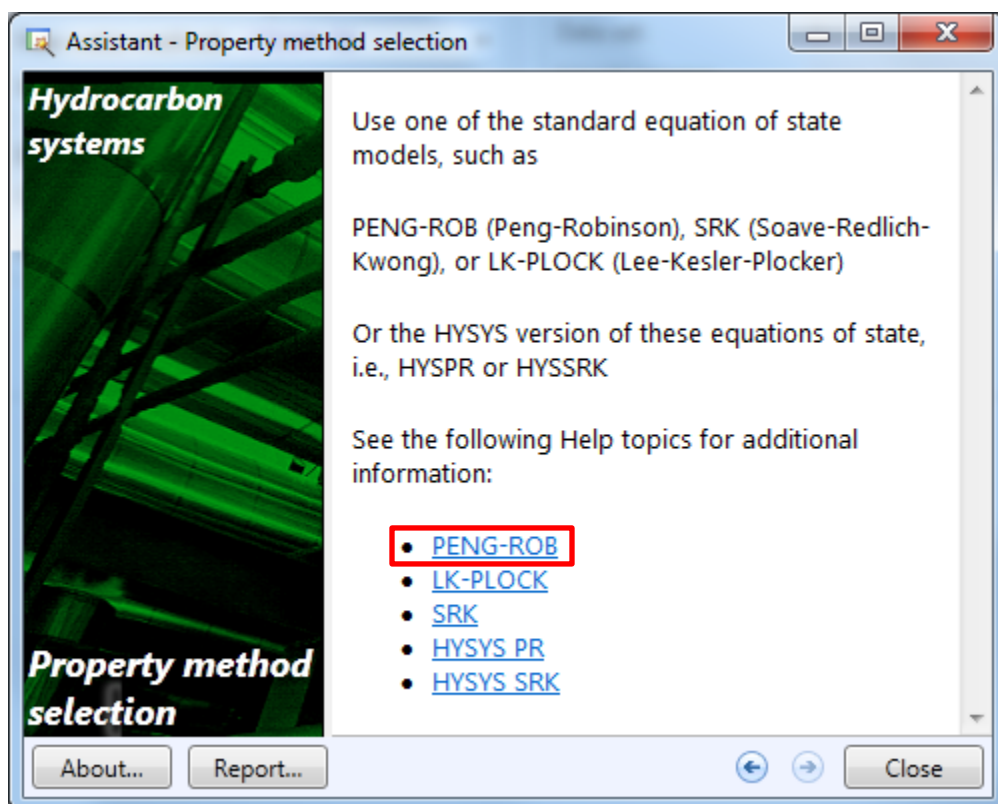
- 4.01. Create a new simulation in Aspen Plus using the **Blank Simulation** template. The **Components | Specification | Selection** sheet is displayed. Enter **ETHYLENE** and **ETHANE** for **Component ID**.

Component ID	Type	Component name	Alias
ETHYLENE	Conventional	ETHYLENE	C2H4
ETHANE	Conventional	ETHANE	C2H6

- 4.02. Go to the **Methods | Specifications | Global** sheet. Click the **Method assistant** button. The Method assistant feature in Aspen Plus helps the user to determine which property method to use for a specific problem.

The screenshot displays the Aspen Plus software interface, specifically the 'Global' sheet under the 'Methods | Specifications' section. The interface is divided into several panels. On the left, there are sections for 'Property methods & options', 'Petroleum calculation options', and 'Electrolyte calculation options'. The 'Property methods & options' section includes dropdowns for 'Method filter' (set to 'COMMON'), 'Base method', and 'Henry components'. The 'Petroleum calculation options' section includes dropdowns for 'Free-water method' (set to 'STEAM-TA') and 'Water solubility' (set to '3'). The 'Electrolyte calculation options' section includes a dropdown for 'Chemistry ID' and a checked checkbox for 'Use true components'. On the right, there is a 'Method name' dropdown and a button labeled 'Methods Assistant...' which is highlighted with a red rectangle. Below the 'Method name' dropdown is a 'Modify' section with a checkbox and several dropdowns for 'EOS', 'Data set', 'Liquid gamma', 'Data set', 'Liquid molar enthalpy', and 'Liquid molar volume'. At the bottom of the 'Modify' section are three checkboxes: 'Heat of mixing', 'Poynting correction', and 'Use liquid reference state enthalpy'.

- 4.03. In the **Assistant – Property method selection** window, select **Next | Specify component type | Hydrocarbon system | No**. The Method assistant will then recommend several methods. In this tutorial, we will use Peng-Robinson for the property method.



- 4.04. Click the **Close** button to exit the methods assistant window. Select **PENG-ROB** for **Base method**.

The screenshot shows the 'Methods Assistant' window with the 'Global' tab selected. The 'Property methods & options' section includes a 'Method filter' set to 'COMMON', a 'Base method' set to 'PENG-ROB', and 'Henry components' set to an empty dropdown. The 'Petroleum calculation options' section has a 'Free-water method' set to 'STEAM-TA' and 'Water solubility' set to '3'. The 'Electrolyte calculation options' section has a 'Chemistry ID' set to an empty dropdown and a checked 'Use true components' checkbox. The 'Method name' dropdown is set to 'PENG-ROB'. The 'Modify' section includes 'EOS' set to 'ESPRSTD', 'Data set' set to '1', 'Liquid gamma' set to an empty dropdown, 'Data set' set to an empty dropdown, 'Liquid molar enthalpy' set to 'HLMX106', and 'Liquid molar volume' set to 'VLMX20'. There are also checkboxes for 'Heat of mixing', 'Poynting correction', and 'Use liquid reference state enthalpy', all of which are unchecked.

- 4.05. In the navigation pane, select **Methods | Parameters | Binary Interaction | PRKBV-1** node to populate binary interaction parameters. This can also be achieved by pressing **F4** key. The binary interaction parameters are displayed on the **Methods | Parameters | Binary Interaction | PRKBV-1 | Input** sheet.

The screenshot shows the 'Input' sheet for the 'PRKBV' parameter. The 'Parameter' dropdown is set to 'PRKBV' and the 'Data set' dropdown is set to '1'. The 'Temperature-dependent binary parameters' section contains a table with the following data:

Parameter	Value
Component i	ETHYLENE
Component j	ETHANE
Temperature units	C
Source	EOS-LIT
Property units	
KAIJ	0.0089
KBIJ	0
KCIJ	0
TLOWER	-273.15
TUPPPER	726.85

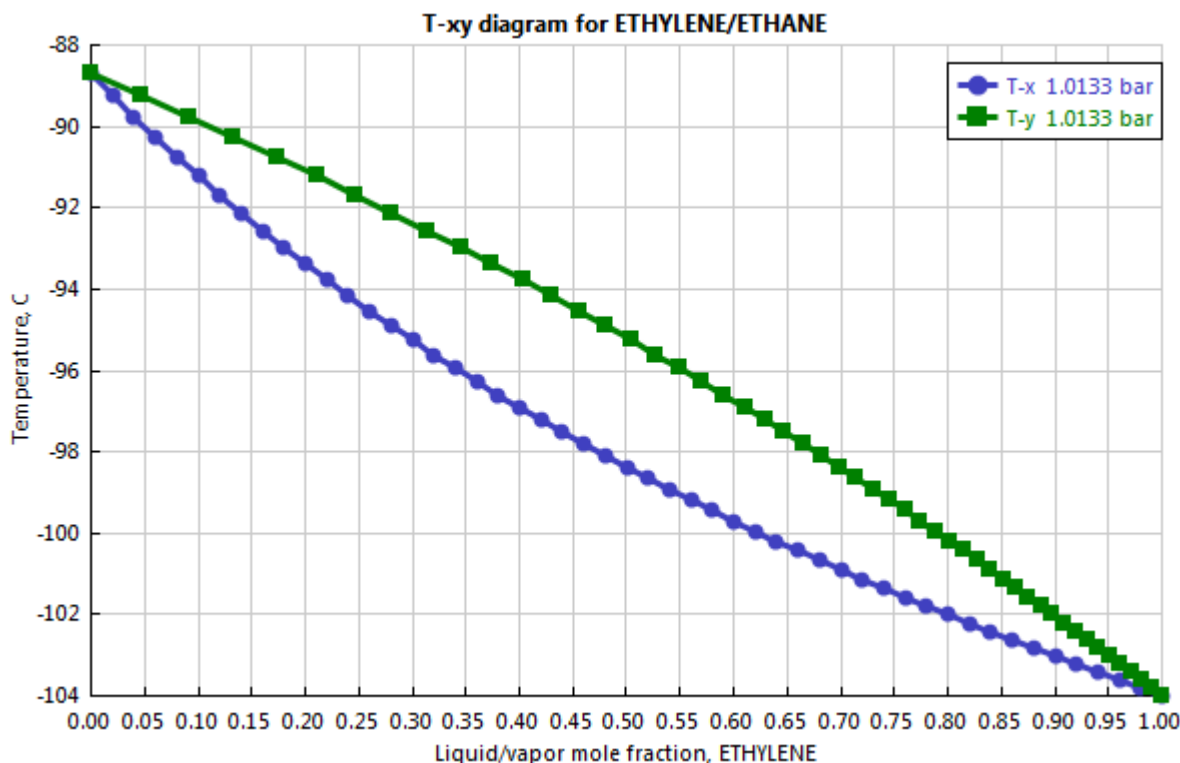
4.06. Click the **Analysis | Binary** button on the **Home** tab of the ribbon.



4.07. The **Analysis | BINRY-1 | Input Binary Analysis** sheet is displayed. Confirm that **Component 1** is **ETHYLENE** and **Component 2** is **ETHANE**.

The image shows a 'Binary Analysis' dialog box with two tabs: 'Binary Analysis' (selected) and 'Diagnostics'. The 'Analysis type' is set to 'Txy'. Under 'Components', 'Component 1' is 'ETHYLENE' and 'Component 2' is 'ETHANE'. Under 'Compositions', 'Basis' is 'Mole fraction' and 'Vary' is 'ETHYLENE'. The 'List of values' radio button is selected for compositions, and the 'Overall range' radio button is selected for the analysis range. The 'Valid phases' dropdown is set to 'Vapor-Liquid'. The 'Pressure' is set to 'bar'. The 'List of values' for pressure is '1.01325'. The 'Overall range' for pressure has a 'Lower limit' of '0' and an 'Upper limit' of '1'. The 'Number of points' is '51' and 'Increments' is empty. The 'Property options' section shows 'Property method' as 'PENG-ROB', 'Henry components' as empty, 'Chemistry ID' as empty, and 'Calculation approach' as 'True components'. A 'Run Analysis' button is at the bottom left.

4.08. Click the **Run analysis** button. The Txy diagram will be generated as shown below.



5. Conclusions

Based on the generated Txy diagram, it should be straightforward to separate ethane and ethylene using distillation. You should now be familiar with how to use the Methods assistant to help select base property methods, and you should be familiar with how to perform a binary analysis to generate Txy diagrams.

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