

# 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

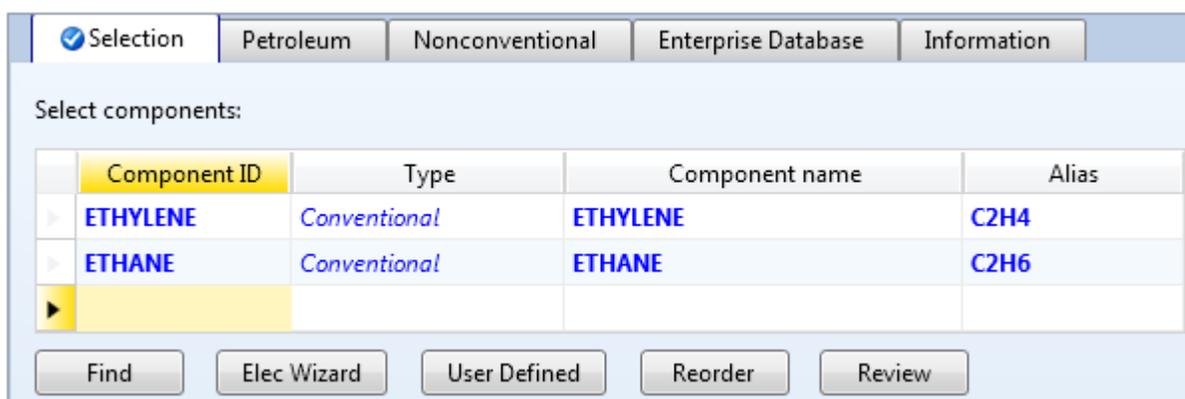
A glance at the Txy diagram for a binary system can quickly tell whether it is easy to separate the two components. If the x-curve and y-curve are not close together and there is no azeotrope, then it is easy to separate the two components using distillation. If there is an azeotrope, then we have to 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**.

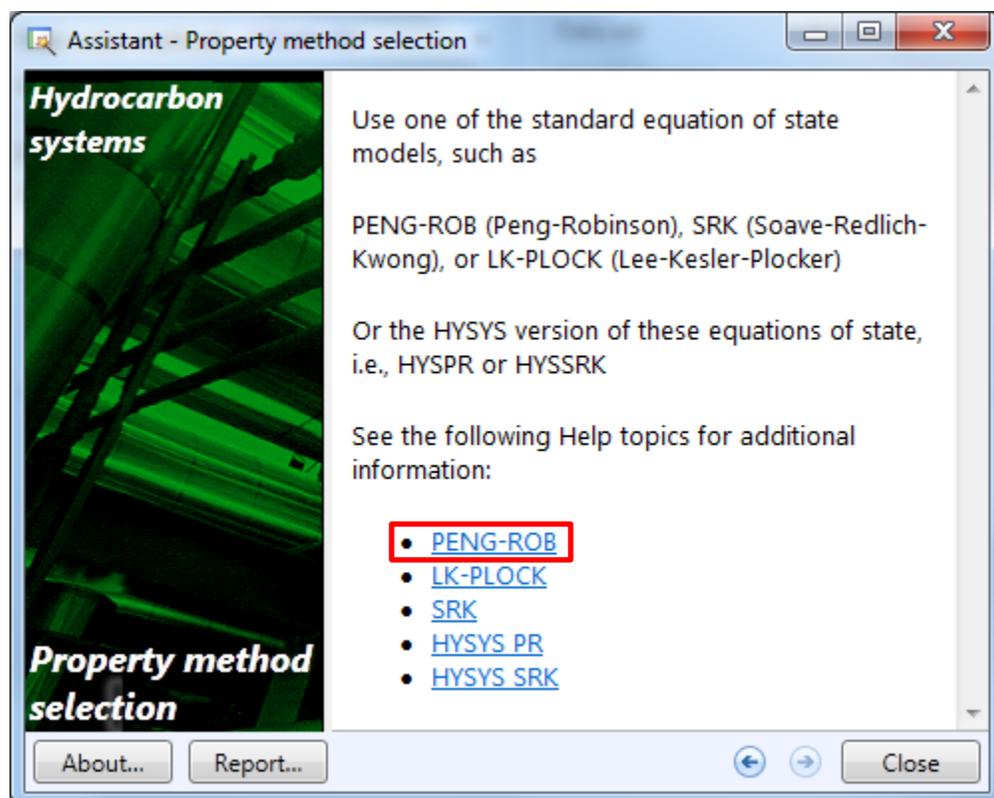


- 4.02. Go to the **Methods | Specifications | Global** sheet. Click the **Method assistant** button. The Method assistant feature in Aspen Plus helps the user to determine which property method to use for a specific problem.

The screenshot displays the 'Global' sheet interface in Aspen Plus. The top navigation bar includes 'Global', 'Flowsheet Sections', 'Referenced', and 'Information'. The main area is divided into several sections:

- Property methods & options:** Includes 'Method filter' (set to COMMON), 'Base method', and 'Henry components'.
- Petroleum calculation options:** Includes 'Free-water method' (set to STEAM-TA) and 'Water solubility' (set to 3).
- Electrolyte calculation options:** Includes 'Chemistry ID' and a checked 'Use true components' checkbox.
- Method name:** A dropdown menu with 'Methods Assistant...' highlighted in a red box.
- Modify:** A section with a checked 'Modify' checkbox and several options: EOS, Data set (1), Liquid gamma, Data set (1), Liquid molar enthalpy, Liquid molar volume, 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**.

Global | Flowsheet Sections | Referenced | Information

Property methods & options

Method filter: COMMON

Base method: **PENG-ROB**

Henry components:

Petroleum calculation options

Free-water method: STEAM-TA

Water solubility: 3

Electrolyte calculation options

Chemistry ID:

Use true components

Method name: **PENG-ROB** Methods Assistant...

Modify

EOS: ESPRSTD

Data set: 1

Liquid gamma:

Data set:

Liquid molar enthalpy: HLMX106

Liquid molar volume: VLMX20

Heat of mixing

Poynting correction

Use liquid reference state enthalpy

- 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.

Input | Databanks | Information

Parameter: PRKBV Data set: 1

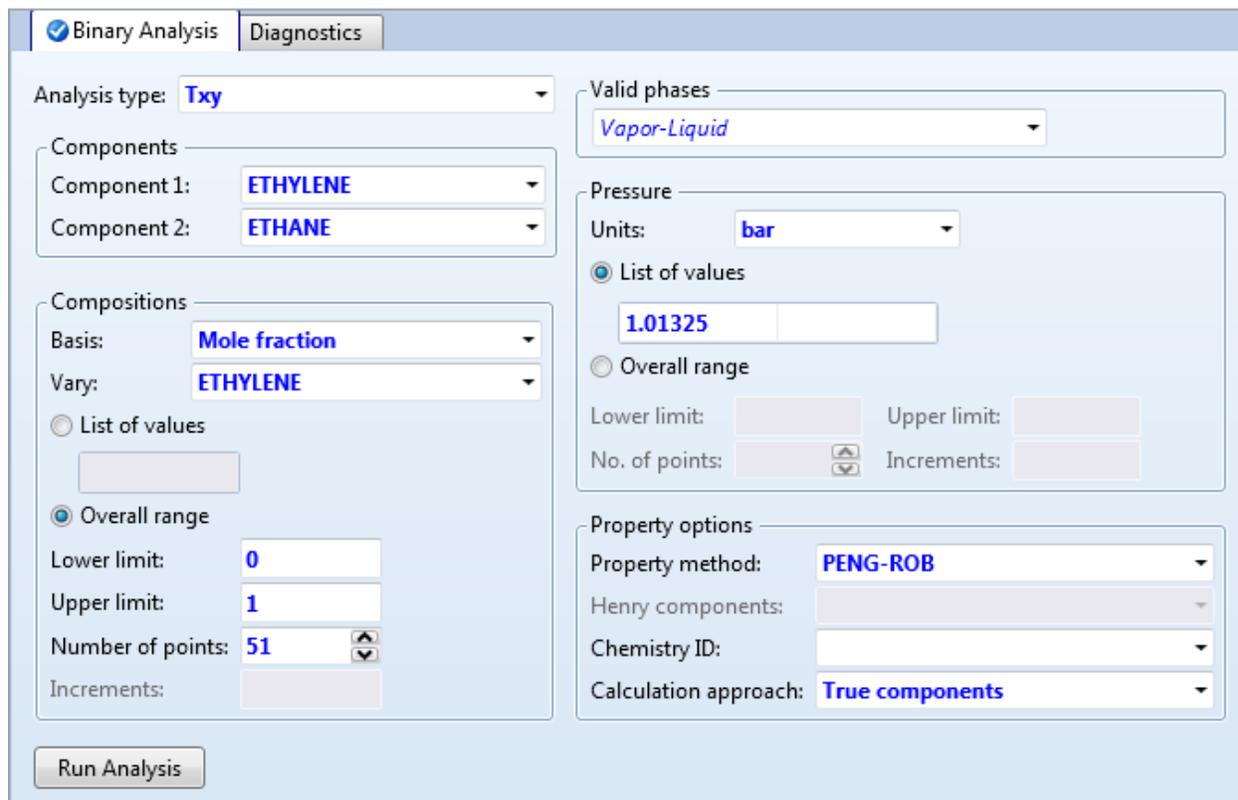
Temperature-dependent binary parameters

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	

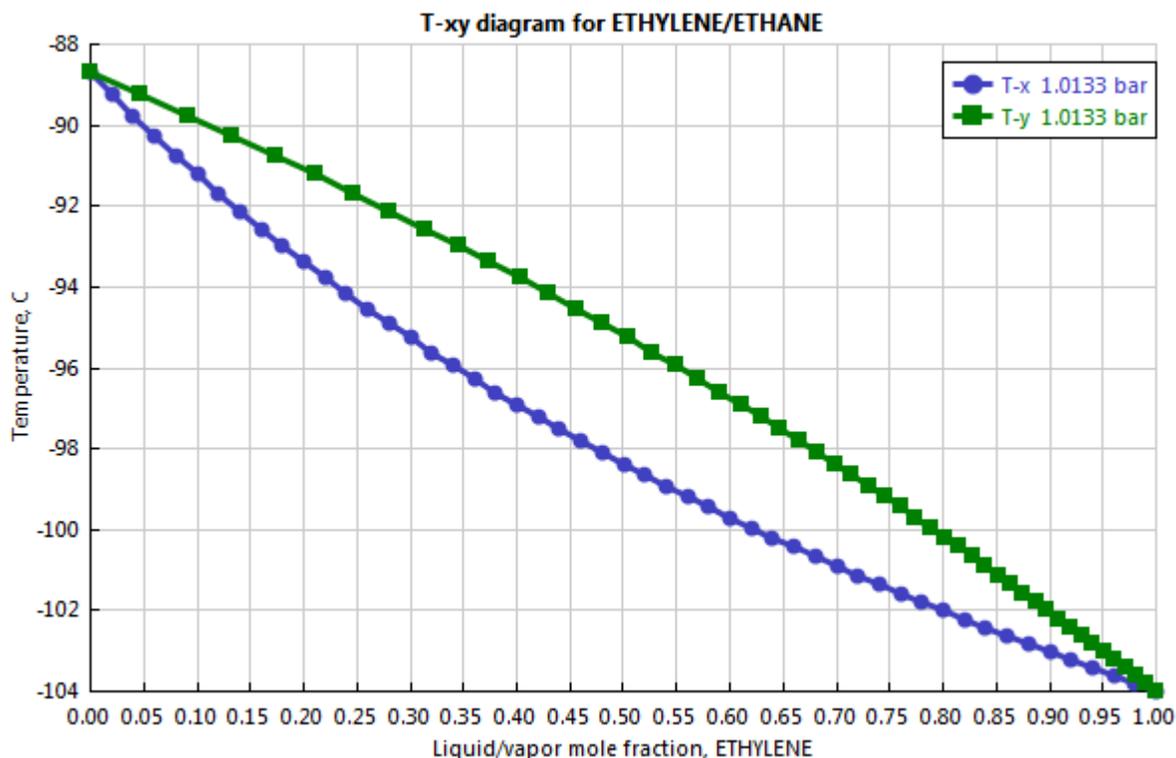
4.06. Click the **Analysis | Binary** button on the **Home** tab of the ribbon.



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

A screenshot of the 'Binary Analysis' dialog box. The 'Binary Analysis' tab is selected. The 'Analysis type' is set to 'Txy'. Under 'Components', 'Component 1' is 'ETHYLENE' and 'Component 2' is 'ETHANE'. Under 'Compositions', the 'Basis' is 'Mole fraction' and 'Vary' is 'ETHYLENE'. The 'Overall range' radio button is selected, with 'Lower limit' at 0, 'Upper limit' at 1, and 'Number of points' at 51. Under 'Valid phases', 'Vapor-Liquid' is selected. Under 'Pressure', 'Units' is 'bar' and 'List of values' is selected with a value of 1.01325. Under 'Property options', 'Property method' is 'PENG-ROB' and 'Calculation approach' is '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.

## 6. Copyright

Copyright © 2012 by Aspen Technology, Inc. ("AspenTech"). All rights reserved. This work may not be reproduced or distributed in any form or by any means without the prior written consent of AspenTech. ASPENTECH MAKES NO WARRANTY OR REPRESENTATION, EITHER EXPRESSED OR IMPLIED, WITH RESPECT TO THIS WORK and assumes no liability for any errors or omissions. In no event will AspenTech be liable to you for damages, including any loss of profits, lost savings, or other incidental or consequential damages arising out of the use of the information contained in, or the digital files supplied with or for use with, this work. This work and its contents are provided for educational purposes only.

AspenTech®, aspenONE®, and the Aspen leaf logo, are trademarks of Aspen Technology, Inc.. Brands and product names mentioned in this documentation are trademarks or service marks of their respective companies.