Ternary Maps for Liquid-Liquid Equilibrium Illustration with Aspen Plus® V8.0

Ethanol-Water-Cyclohexane System

1. Lesson Objectives

- Learn how to generate ternary maps in Aspen Plus for systems with two liquid phases

2. Prerequisites

- Aspen Plus V8.0

3. Background

Ternary maps provide a clear picture of Liquid-Liquid Equilibrium (LLE) for a ternary system and are a very useful tool for process design. For example, the ternary system of water, ethanol and cyclohexane forms three binary azeotropes and one ternary azeotrope (0.1609, 0.3058, and 0.533 in mole fraction, respectively). These azeotropes divide composition space into multiple distillation regions and make it very difficult to separate these components into pure components if we only use one distillation. Liquid-liquid separation using a decanter is a very effective way to cross distillation boundaries in azeotropic distillation processes. Ternary maps show us whether and how LLE can be leveraged in separation process design.

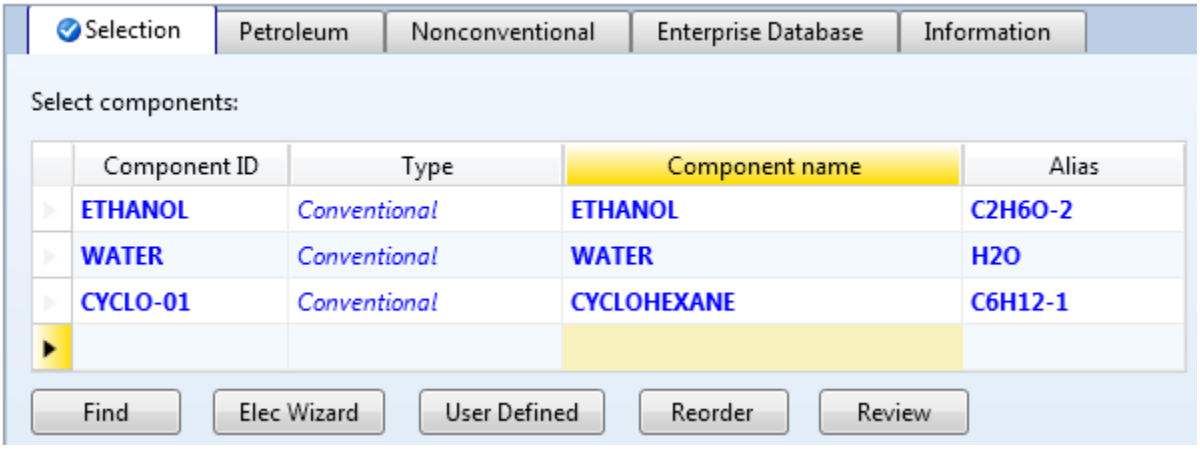
The examples presented are solely intended to illustrate specific concepts and principles. They may not reflect an industrial application or real situation.

4. Aspen Plus Solution

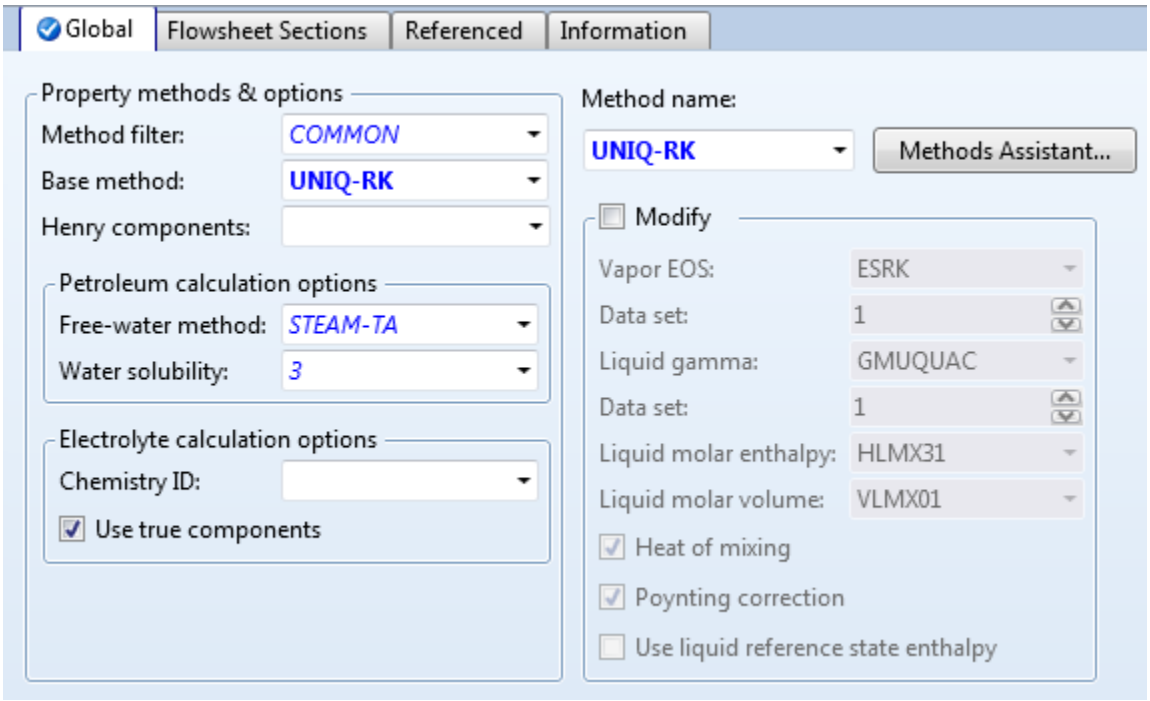
If you are unfamiliar with how to start Aspen Plus, select components, or define methods, consult **Get Started Guide for New Users of Aspen Plus.pdf** for instructions.

4.01. Start a new simulation using the **Blank Simulation** template in Aspen Plus.

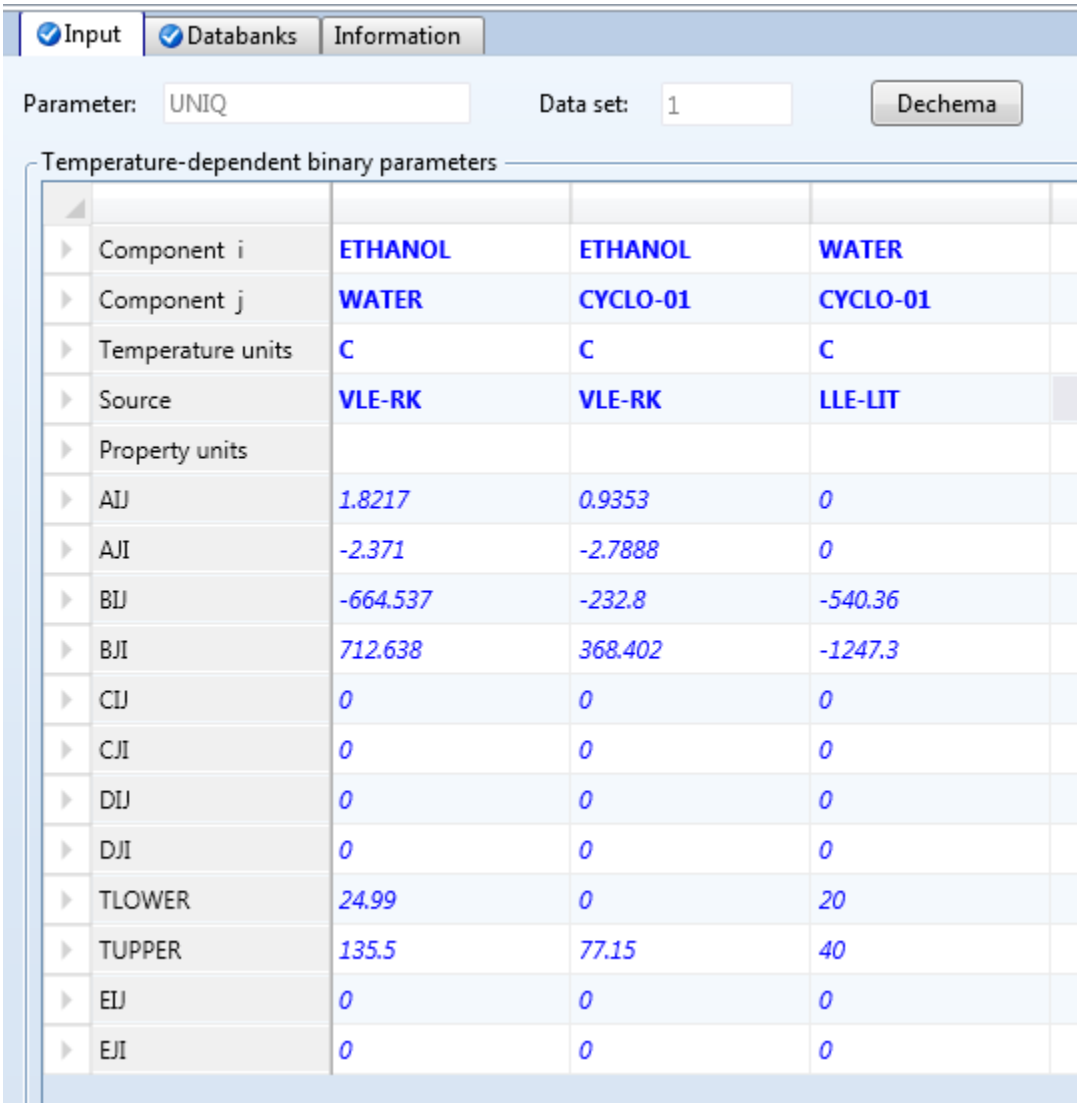
4.02. The **Components | Specification | Selection** sheet is displayed. Enter **ETHANOL**, **WATER**, and **CYCLO-01** for **Component ID**. Enter **CYCLOHEXANE** in the **Component name** column for component **CYCLO-01**.



4.03. Go to the **Methods | Specifications | Global** sheet**.** Select **UNIQ-RK** for **Method name**. The UNIQ-RK model uses the UNIQUAC model for the liquid phase and uses the Redlich-Kwong equation of state to model the vapor phase.

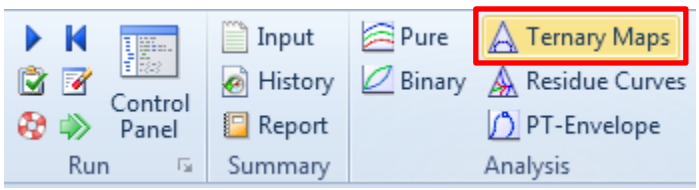


4.04. Retrieve binary interaction parameters. Click the **Next** button (or press the **F4 key**) or navigate to the **Methods | Parameters | Binary Interaction | UNIQ-1 | Input** sheet. The binary parameters are filled automatically.

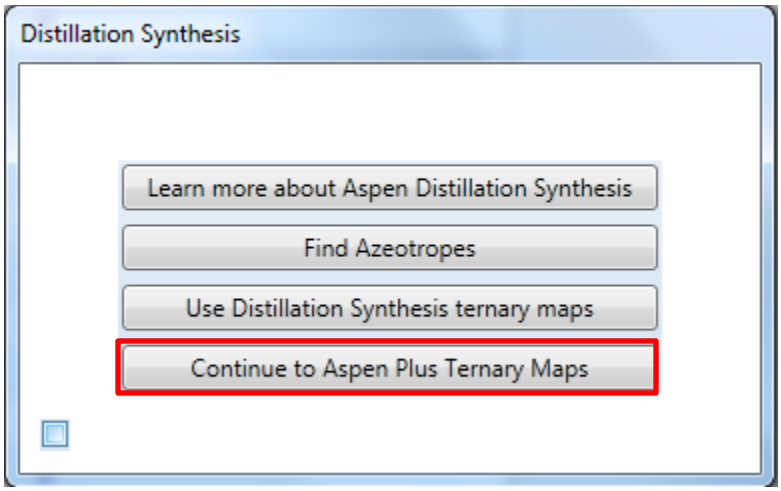


Component i	ETHANOL	ETHANOL	WATER
Component j	WATER	CYCLO-01	CYCLO-01
Temperature units	C	C	C
Source	VLE-RK	VLE-RK	LLE-LIT
Property units			
AIJ	1.8217	0.9353	0
AJI	-2.371	-2.7888	0
BIJ	-664.537	-232.8	-540.36
BJI	712.638	368.402	-1247.3
CIJ	0	0	0
CJI	0	0	0
DIJ	0	0	0
DJI	0	0	0
TLOWER	24.99	0	20
TUPPER	135.5	77.15	40
EIJ	0	0	0
EJI	0	0	0

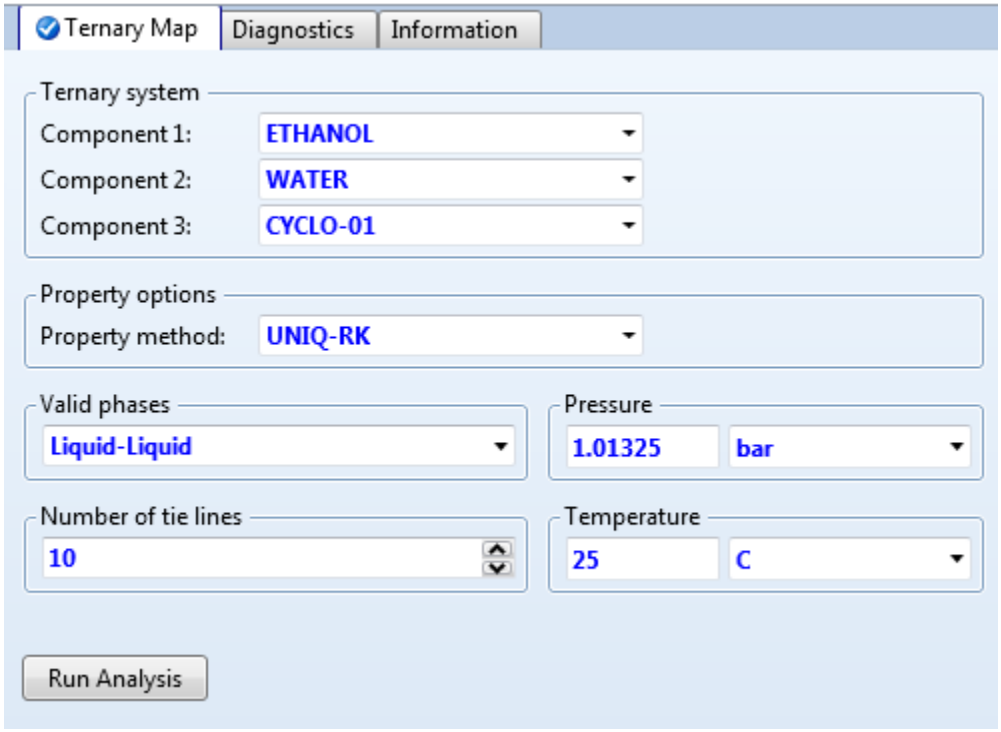
4.05. Create a ternary map. From the **Home** tab of the ribbon, click the **Analysis | Ternary Maps** button.



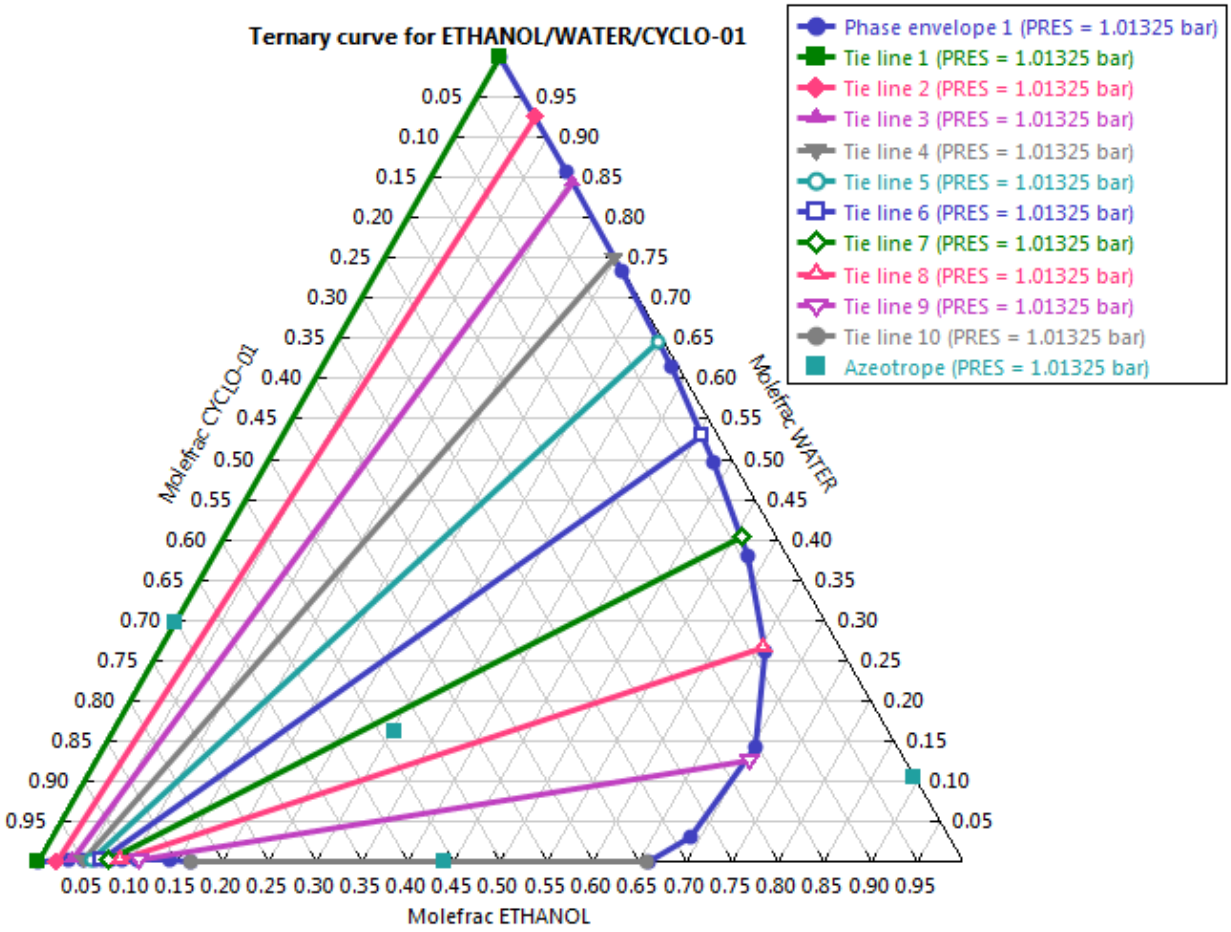
4.06. The **Distillation Synthesis** window pops up.



4.07. Click the **Continue to Aspen Plus Ternary Maps** button. The **Analysis | TERDI-1 | Input | Ternary Map** sheet is displayed. Select **Liquid-Liquid** for **Valid phases**. Enter **10** for **Number of tie lines** and **25** for **Temperature**.



4.08. Click the **Run analysis** button. A ternary diagram is generated as shown below.



4.09. The squares on the diagram represent the compositions of azeotropes. There are 3 binary azeotropes and 1 ternary azeotrope. The phase envelope line represents the liquid-liquid equilibrium compositions.

5. Conclusions

Liquid-liquid separation using a decanter is an effective way to cross distillation regions for azeotropic distillation process synthesis and ternary maps provide a full and clear picture on liquid-liquid equilibrium for ternary systems. Therefore, ternary maps are very important for synthesis and design of separation processes.

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