

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**.

The screenshot shows the 'Selection' sheet in Aspen Plus. The 'Component name' column for 'CYCLO-01' is highlighted in yellow, indicating the entry 'CYCLOHEXANE'.

Component ID	Type	Component name	Alias
ETHANOL	Conventional	ETHANOL	C2H6O-2
WATER	Conventional	WATER	H2O
CYCLO-01	Conventional	CYCLOHEXANE	C6H12-1

- 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.

The screenshot shows the 'Global' sheet in Aspen Plus. The 'Method name' is set to 'UNIQ-RK'. The 'Modify' section is expanded, showing various options for the method.

Property methods & options

- Method filter: COMMON
- Base method: UNIQ-RK
- Henry components:

Petroleum calculation options

- Free-water method: STEAM-TA
- Water solubility: 3

Electrolyte calculation options

- Chemistry ID:
- Use true components

Method name: UNIQ-RK

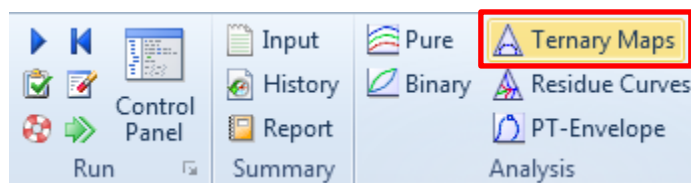
Modify

- Vapor EOS: ESRK
- Data set: 1
- Liquid gamma: GMUQUAC
- Data set: 1
- Liquid molar enthalpy: HLMX31
- Liquid molar volume: VLMX01
- Heat of mixing
- Poynting correction
- Use liquid reference state enthalpy

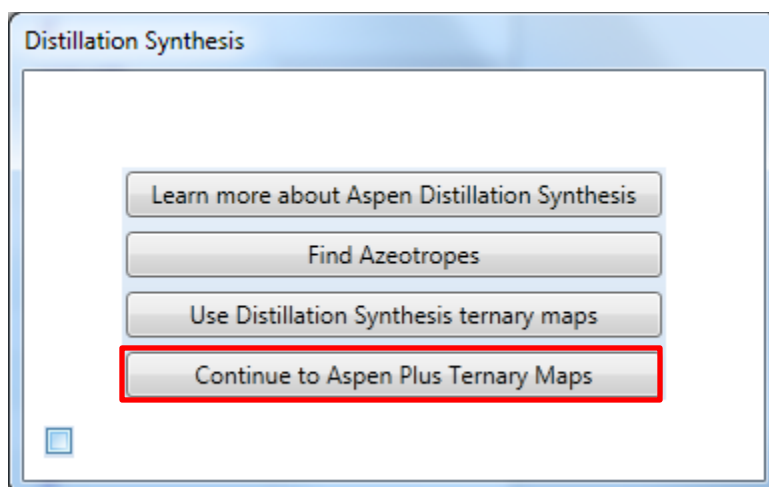
- 4.04. Retrieve binary interaction parameters. Click the **Next** button (or press the **F4 key**) or navigate to the **Methods | Parameters | Binary Interaction | UNIQ-1 | Input** sheet. The binary parameters are filled automatically.

<input checked="" type="checkbox"/> Input <input checked="" type="checkbox"/> Databanks Information					
Parameter:		UNIQ	Data set:	1	Dechema
Temperature-dependent binary parameters					
▶ 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		

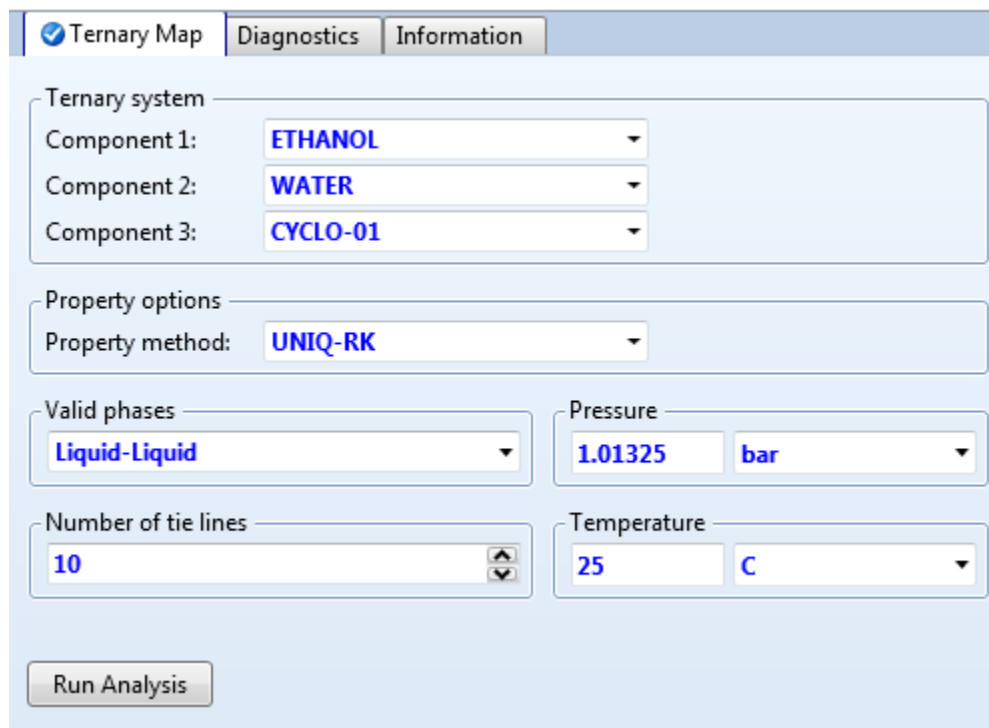
- 4.05. Create a ternary map. From the **Home** tab of the ribbon, click the **Analysis | Ternary Maps** button.



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**.



Analysis | TERDI-1 | Input | Ternary Map

Ternary Map | Diagnostics | Information

Ternary system

Component 1: ETHANOL

Component 2: WATER

Component 3: CYCLO-01

Property options

Property method: UNIQ-RK

Valid phases: Liquid-Liquid

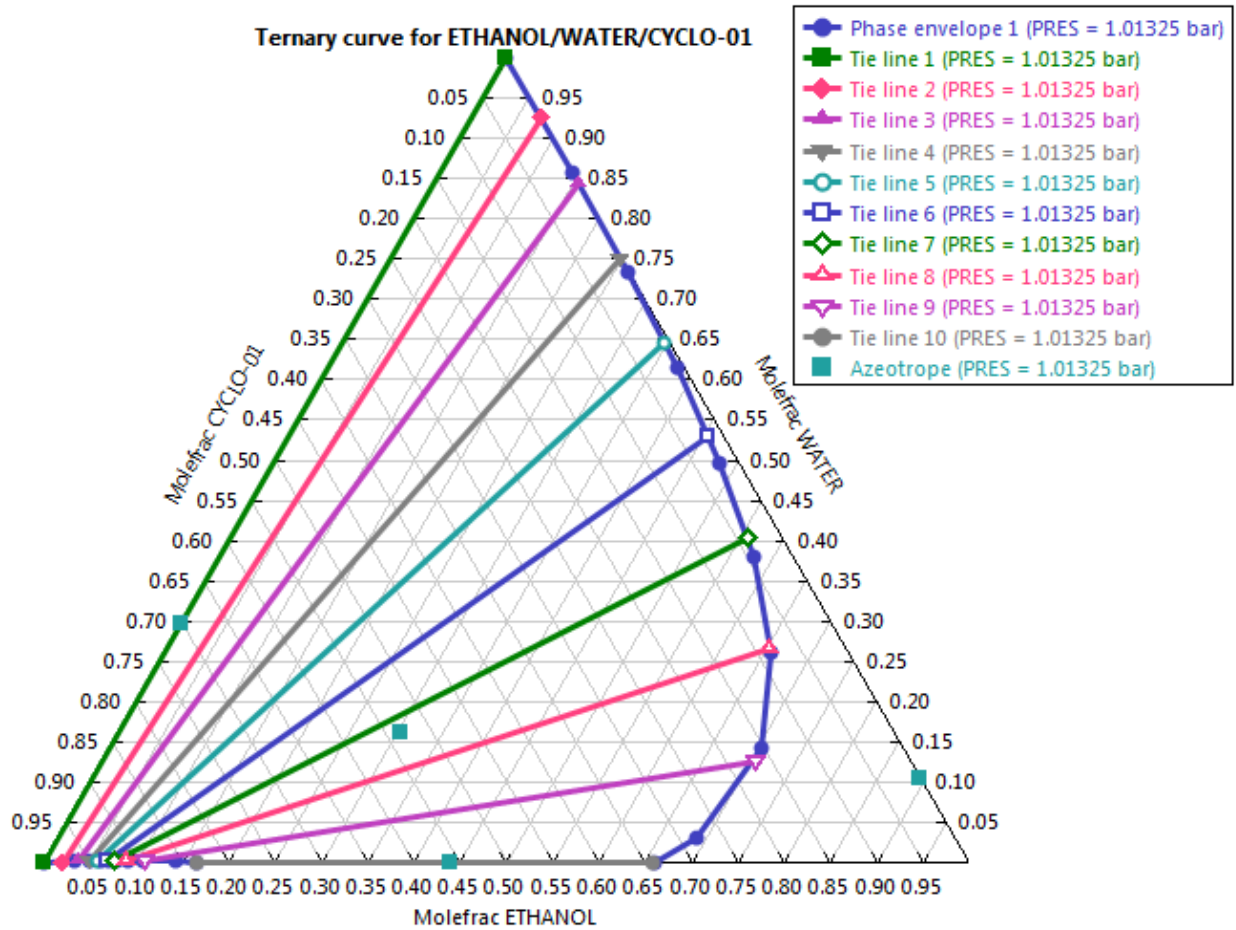
Pressure: 1.01325 bar

Number of tie lines: 10

Temperature: 25 C

Run Analysis

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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