

Txy Examples for VLLE systems with Aspen Plus® V8.0

1. Lesson Objectives

- Become familiar with Txy diagrams involving vapor-liquid-liquid (VLLE) equilibrium

2. Prerequisites

- Aspen Plus V8.0

3. Background

Water and many organic components are immiscible or partially miscible. This can be leveraged in separation processes. Sometimes a liquid-liquid extraction process is more efficient than a distillation process because we don't need to vaporize as much liquid in liquid-liquid extraction processes. In this tutorial, we will examine the binary systems of water and cyclohexane, water and 3-methyl-hexane, and water and n-butanol.

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 **WATER**, **CYCLO-HE**, **N-BUTANO**, and **C7H16-3** for **Component ID**. Also, enter **CYCLOHEXANE** and **N-BUTANOL** for **Component name** for **CYCLO-HE** and **N-BUTANO**, respectively.

The screenshot shows the 'Selection' sheet in Aspen Plus. The 'Selection' tab is active, and the 'Petroleum' sub-tab is selected. The 'Select components:' section contains a table with the following data:

Component ID	Type	Component name	Alias
WATER	Conventional	WATER	H2O
CYCLO-HE	Conventional	CYCLOHEXANE	C6H12-1
N-BUTANO	Conventional	N-BUTANOL	C4H100-1
C7H16-3	Conventional	3-METHYLHEXANE	C7H16-3

Below the table are several buttons: Find, Elec Wizard, User Defined, Reorder, and Review.

- 4.02. Define methods. Go to the **Methods | Specifications** sheet. Select **UNIQUAC** for **Base method** and click the **Next Input** button (or press **F4**) to populate the binary interaction parameters.

The screenshot displays the 'Methods | Specifications' sheet in a software application. The interface is organized into several sections:

- Global** (selected), **Flowsheet Sections**, **Referenced**, and **Information** tabs are visible at the top.
- Property methods & options**:
 - Method filter: COMMON
 - Base method: UNIQUAC
 - Henry components: (empty)
- Petroleum calculation options**:
 - Free-water method: STEAM-TA
 - Water solubility: 3
- Electrolyte calculation options**:
 - Chemistry ID: (empty)
 - Use true components
- Method name**: UNIQUAC (with a 'Methods Assistant...' button)
- Modify** section (checkbox):
 - Vapor EOS: ESIG
 - Data set: 1
 - Liquid gamma: GMUQUAC
 - Data set: 1
 - Liquid molar enthalpy: HLMX88
 - Liquid molar volume: VLMX01
 - Heat of mixing
 - Poynting correction
 - Use liquid reference state enthalpy

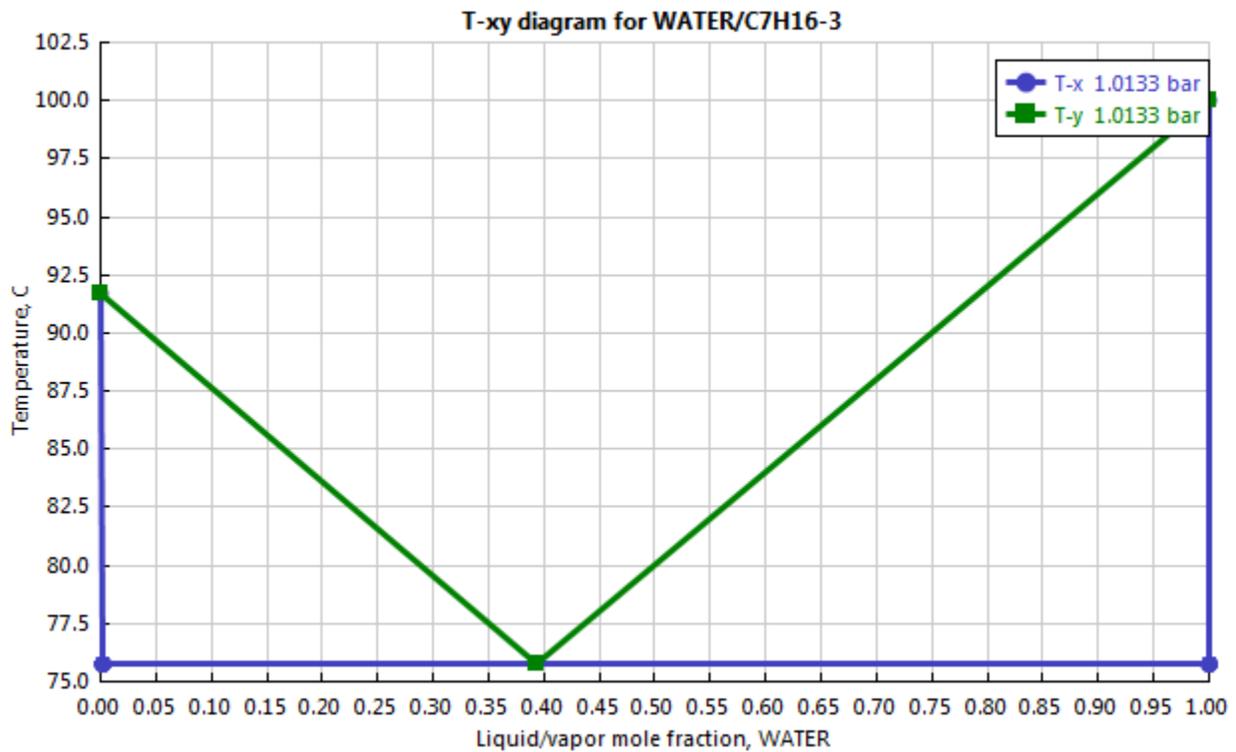
- 4.03. Click the **Analysis | Binary** button on the **Home** tab of the ribbon. The **Analysis | BINRY-1 | Input | Binary Analysis** sheet is displayed. Ensure that **WATER** is selected for **Component 1**. Select **C7H16-3** for **Component 2**. In the **Valid phases** frame, select **Vapor-Liquid-Liquid**.

The screenshot displays the 'Binary Analysis' software interface. At the top, there are two tabs: 'Binary Analysis' (selected) and 'Diagnostics'. The interface is divided into several sections:

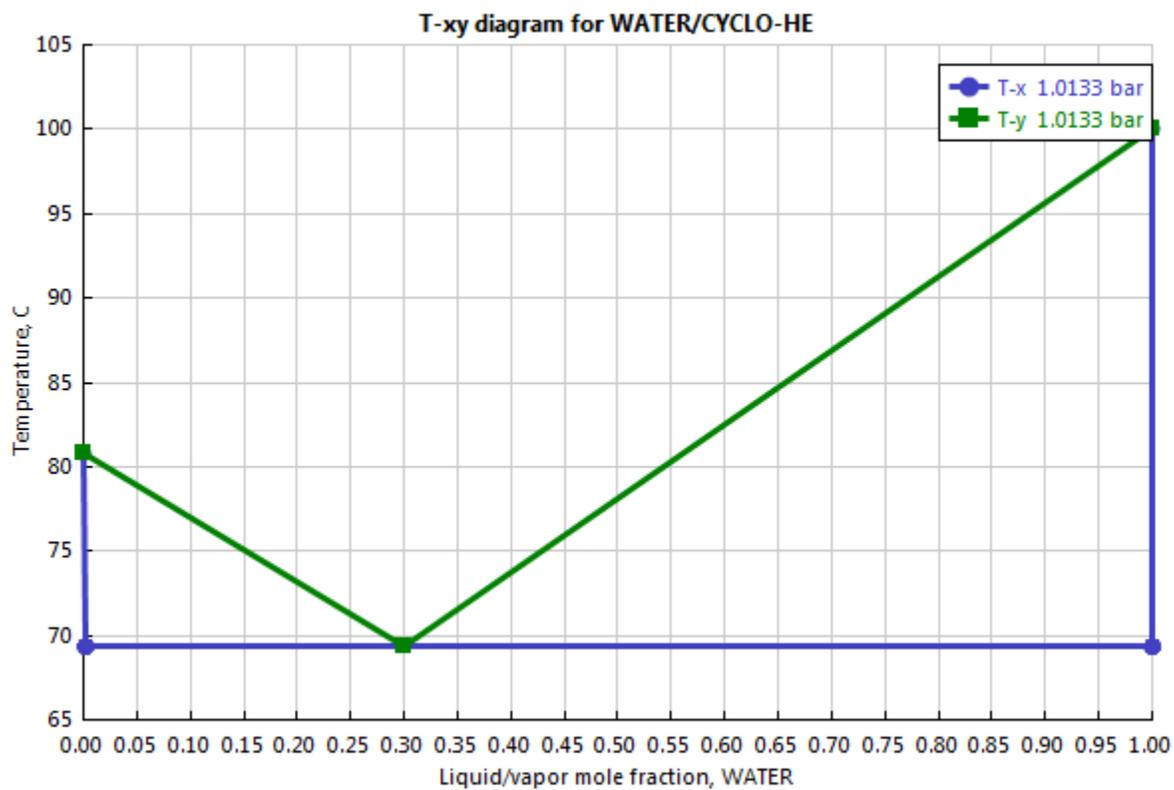
- Analysis type:** A dropdown menu set to 'Txy'.
- Components:** Two dropdown menus. 'Component 1' is set to 'WATER' and 'Component 2' is set to 'C7H16-3'.
- Compositions:** A dropdown menu for 'Basis' set to 'Mole fraction' and another for 'Vary' set to 'WATER'. Below these are two radio buttons: 'List of values' (unselected) and 'Overall range' (selected). Under 'Overall range', there are input fields for 'Lower limit' (0), 'Upper limit' (1), 'Number of points' (51), and 'Increments'.
- Valid phases:** A dropdown menu set to 'Vapor-Liquid-Liquid', which is highlighted with a red rectangular box.
- Pressure:** A dropdown menu for 'Units' set to 'bar'. Below it are two radio buttons: 'List of values' (selected) and 'Overall range' (unselected). Under 'List of values', there is an input field for '1.01325'. Below these are input fields for 'Lower limit', 'Upper limit', 'No. of points', and 'Increments'.
- Property options:** A dropdown menu for 'Property method' set to 'UNIQUAC'. Below it are dropdown menus for 'Henry components' and 'Chemistry ID'. At the bottom is a dropdown menu for 'Calculation approach' set to 'True components'.

At the bottom left of the interface is a button labeled 'Run Analysis'.

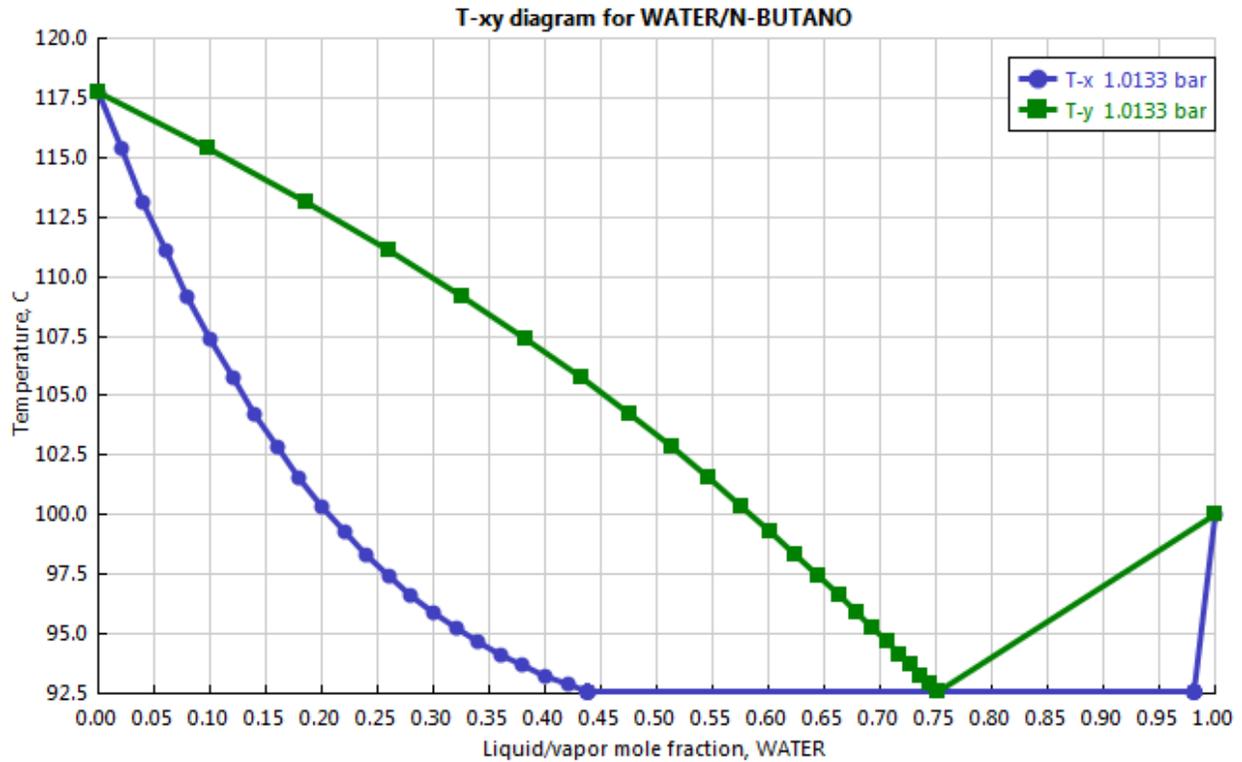
- 4.04. Click the **Run analysis** button. A Txy diagram for the water/3-methylhexane binary system is generated as shown below. Note that there are four regions. In the region above the green lines, only vapor phase exists. In the region within the left triangle, a vapor phase and a liquid phase that contains almost pure 3-methylhexane can exist. In the region within the right triangle, a vapor phase and a liquid phase that contains almost pure water can exist. Below the horizontal blue line is the two liquid phase region where a liquid phase contains almost pure 3-methylhexane and the other liquid phase contains almost pure water. Therefore, the diagram tells us that 3-methylhexane and water are almost completely immiscible. This immiscibility can be leveraged during separation process design (e.g., extraction and heterogeneous azeotropic distillation).



- 4.05. If we perform a similar binary analysis for the water/cyclohexane system, we will get the following T-xy diagram. Note that water and cyclohexane are also almost completely immiscible. As a matter of fact, water is immiscible or partially immiscible with many paraffin components.



- 4.06. If we perform a similar binary analysis for the water/n-butanol system, we will get the following T-xy diagram. Note that water and n-butanol are partially miscible and two liquid phases exist in certain composition range. This behavior can also be leveraged during separation process design involving heterogeneous azeotropic distillation.



5. Conclusions

From the generated Txy diagrams for various binary systems involving vapor-liquid-liquid equilibrium, we can observe that water and some compounds are almost completely immiscible. For instance, water and cyclohexane are almost completely immiscible. Also, water and 3-methyl-hexane are also almost completely immiscible whereas water and n-butanol are partially miscible. Therefore, components such as cyclohexane and 3-methyl-hexane can be very effective solvents for extraction and azeotropic distillation.

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