# 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

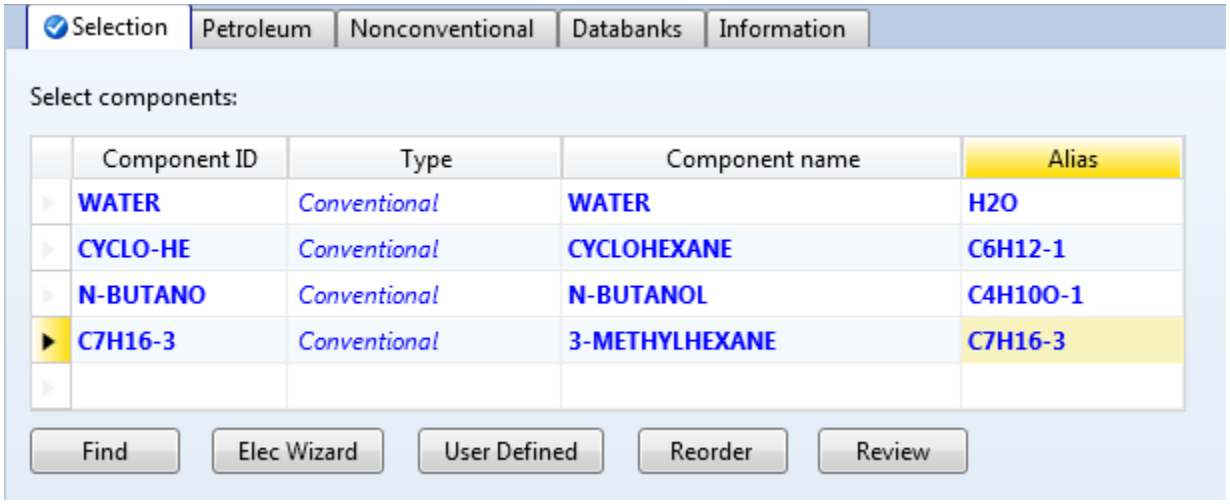
Water and many organic components are immiscible or partially miscible. This can be leveraged in separation processes. Sometimes a liquid-liquid extraction process is more efficient than a distillation process because we don't need to vaporize as much liquid in liquid-liquid extraction processes. In 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.**

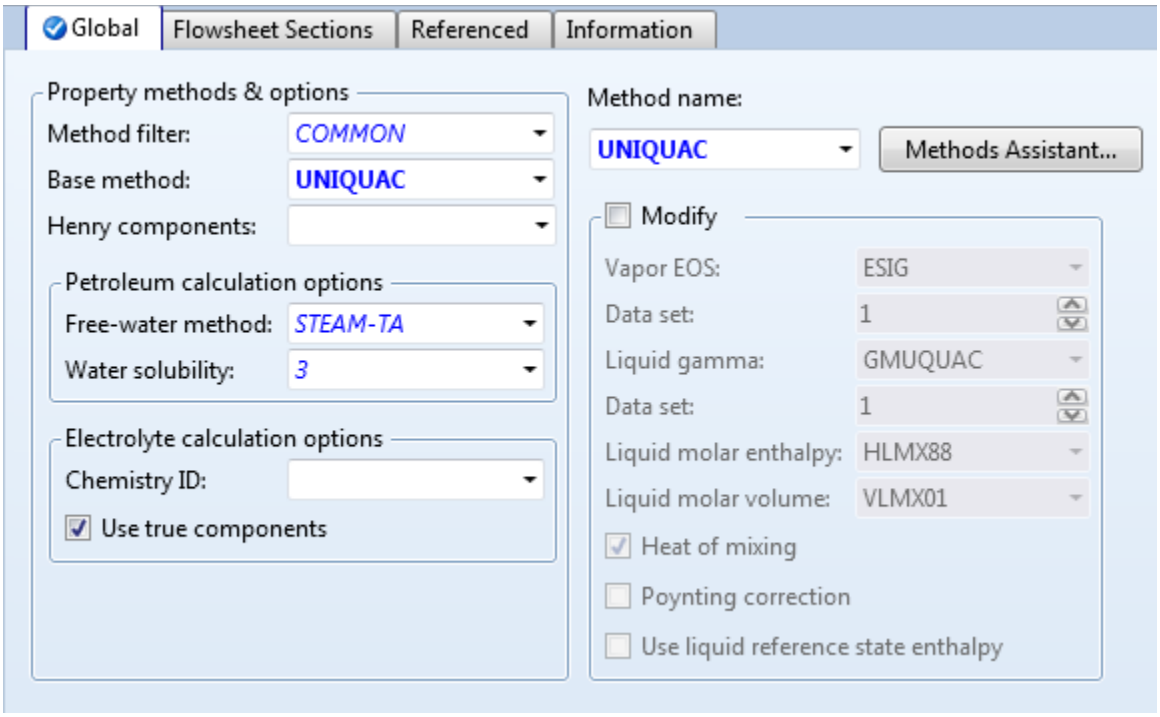
## 4. Aspen Plus Solution

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.

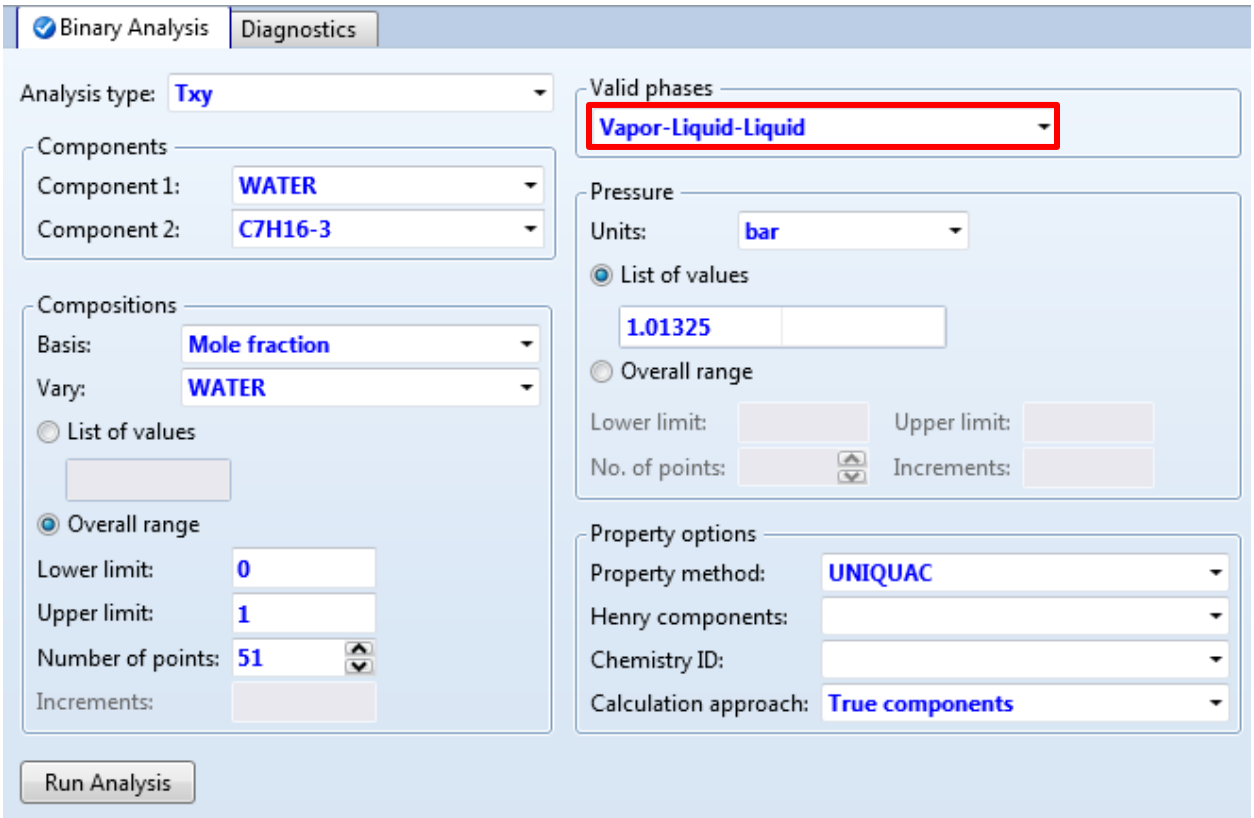
4.01. Create a new simulation in Aspen Plus using the **Blank Simulation** template. The **Components | Specification | Selection** sheet is displayed. Enter **WATER**, **CYCLO-HE**, **N-BUTANO**, and **C7H16-3** for **Component ID**. Also, enter **CYCLOHEXANE** and **N-BUTANOL** for **Component name** for **CYCLO-HE** and **N-BUTANO**, respectively.



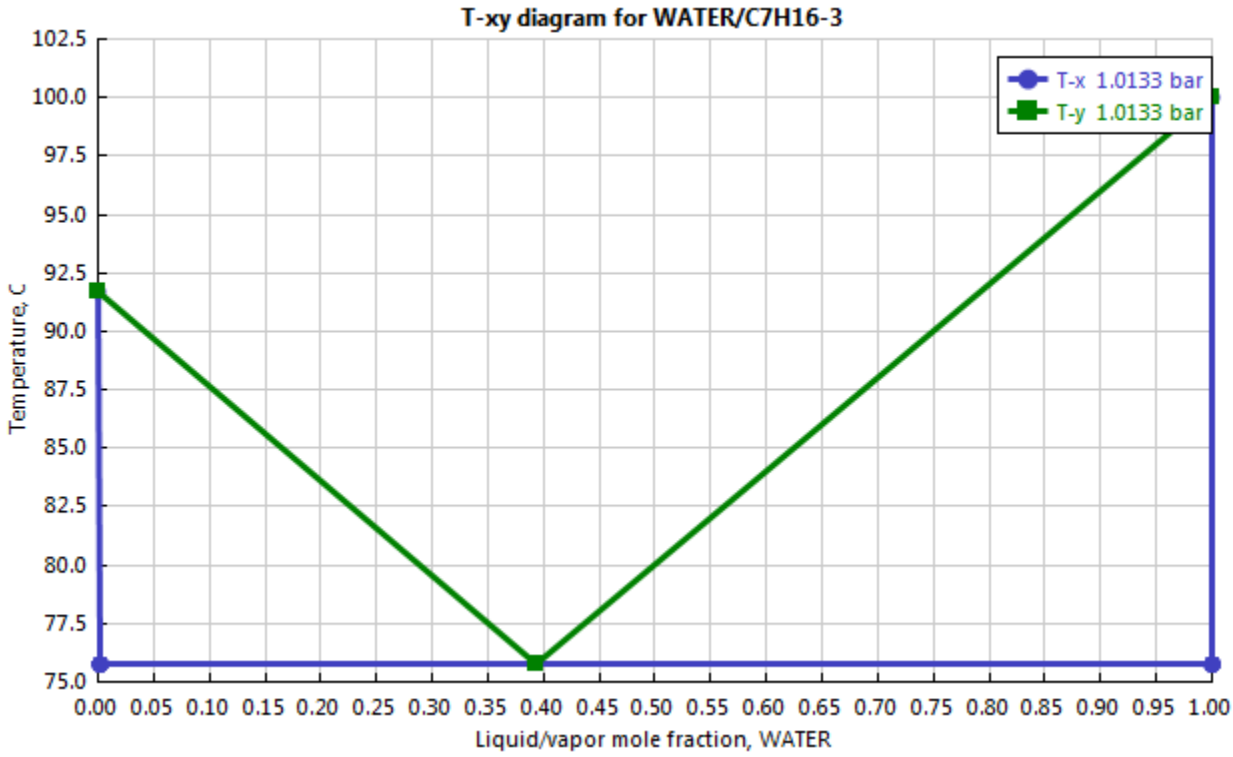
4.02. Define methods. Go to the **Methods | Specifications** sheet. Select **UNIQUAC** for **Base method** and click the **Next Input** button (or press **F4**) to populate the binary interaction parameters.



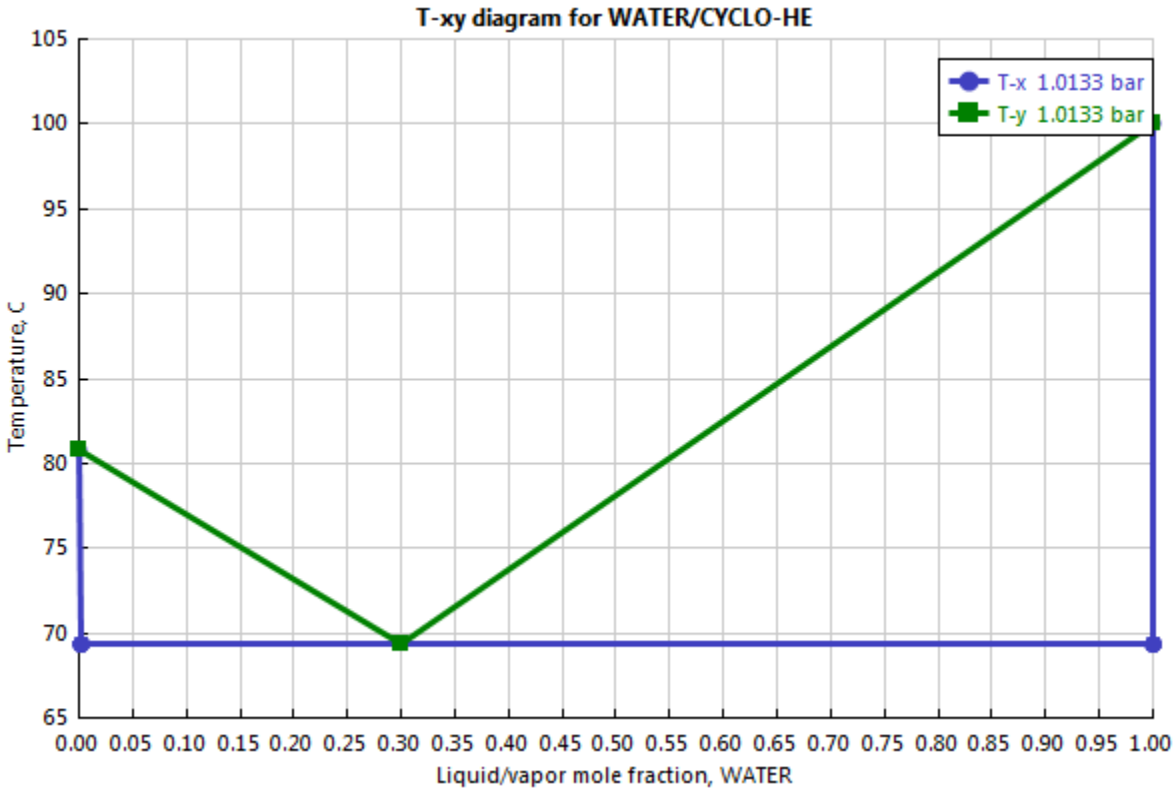
4.03. Click the **Analysis | Binary** button on the **Home** tab of the ribbon. The **Analysis | BINRY-1 | Input | Binary Analysis** sheet is displayed. Ensure that **WATER** is selected for **Component 1**. Select **C7H16-3** for **Component 2**. In the **Valid phases** frame, select **Vapor-Liquid-Liquid**.



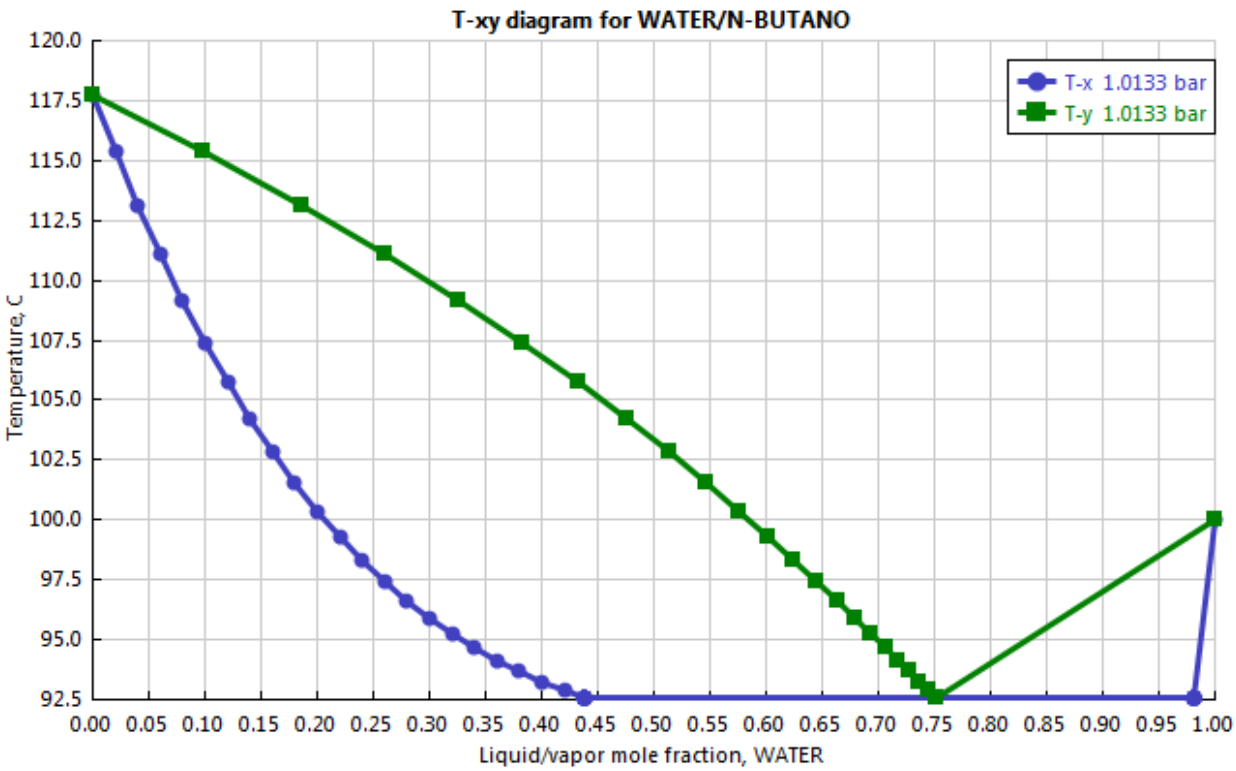
4.04. Click the **Run analysis** button. A Txy diagram for the water/3-methylhexane binary system is generated as shown below. Note that there are four regions. In the region above the green lines, only vapor phase exists. In the region within the left triangle, a vapor phase and a liquid phase that 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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