# Heat of Vaporization with Aspen Plus® V8.0

## 1. Lesson Objectives

- Learn how to calculate heat of vaporization using the **Flash2** block in Aspen Plus
- Understand the impact of heat of vaporization on distillation

## 2. Prerequisites

- Aspen Plus V8.0

## 3. Background

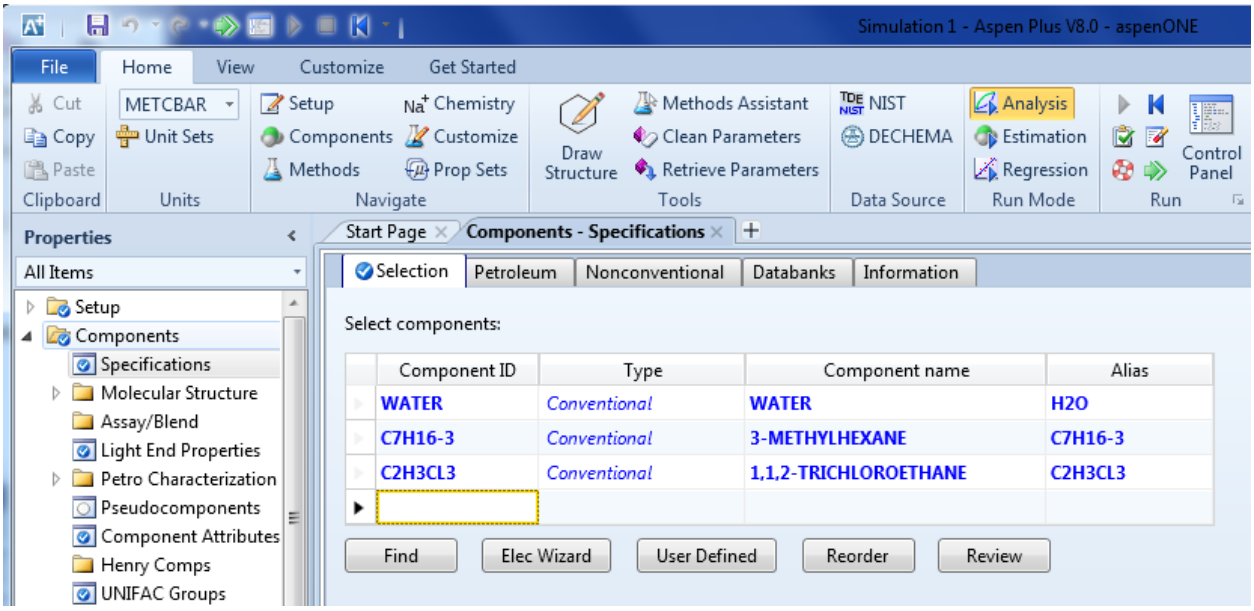
The driving force for distillation is energy. The most energy consuming part of a distillation column is the vaporization of material in the reboiler to cause vapor to flow from the bottom of the column to the top of the column. Heat of vaporization determines the amount of energy required. Therefore, it is important to know the heat of vaporization of various species during solvent selection. With everything else equal, we should select a component with lower heat of vaporization so that we can achieve the same degree of separation with less energy. Example Dist-009 shows that we can achieve significant energy savings by using a solvent with lower heat of vaporization. This example contains three isolated **Flash2** blocks. Each **Flash2** block is used to calculate the heat of vaporization for a pure component.

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

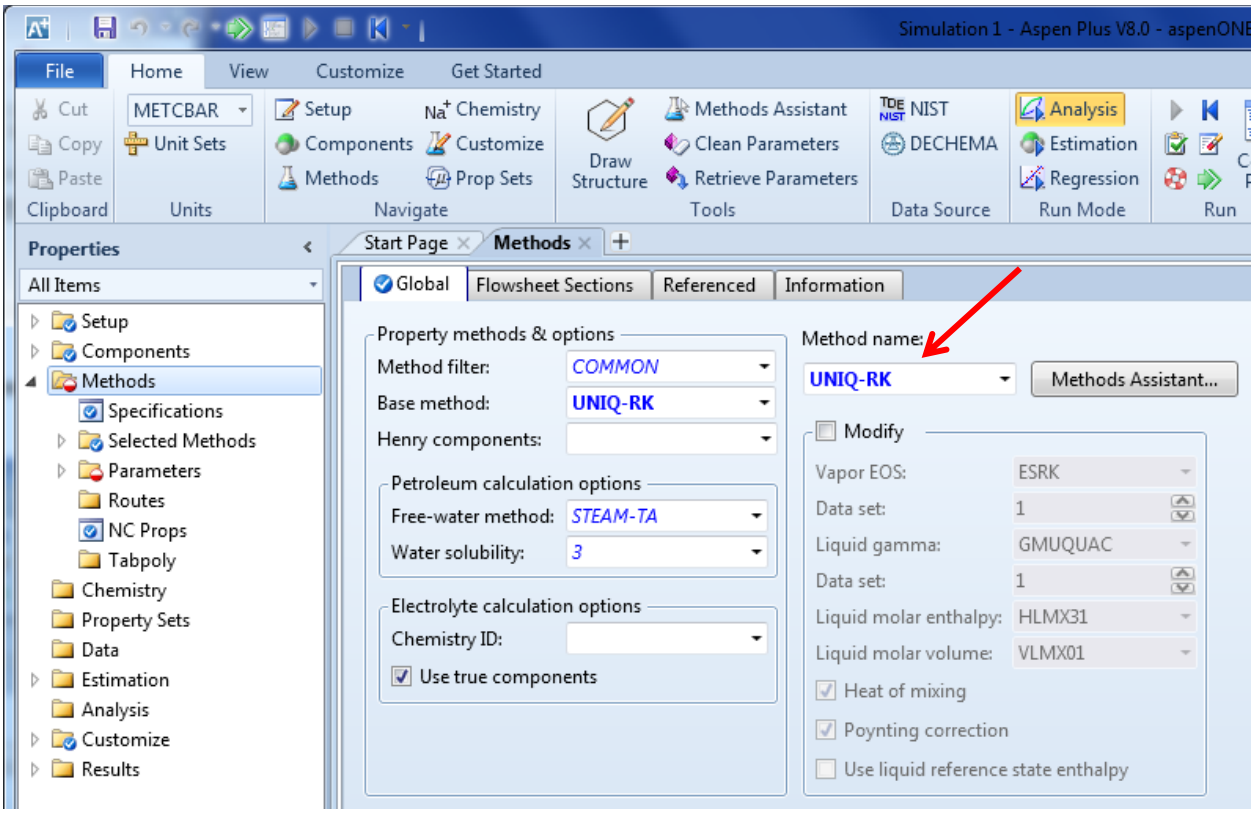
## 4. Aspen Plus Solution

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

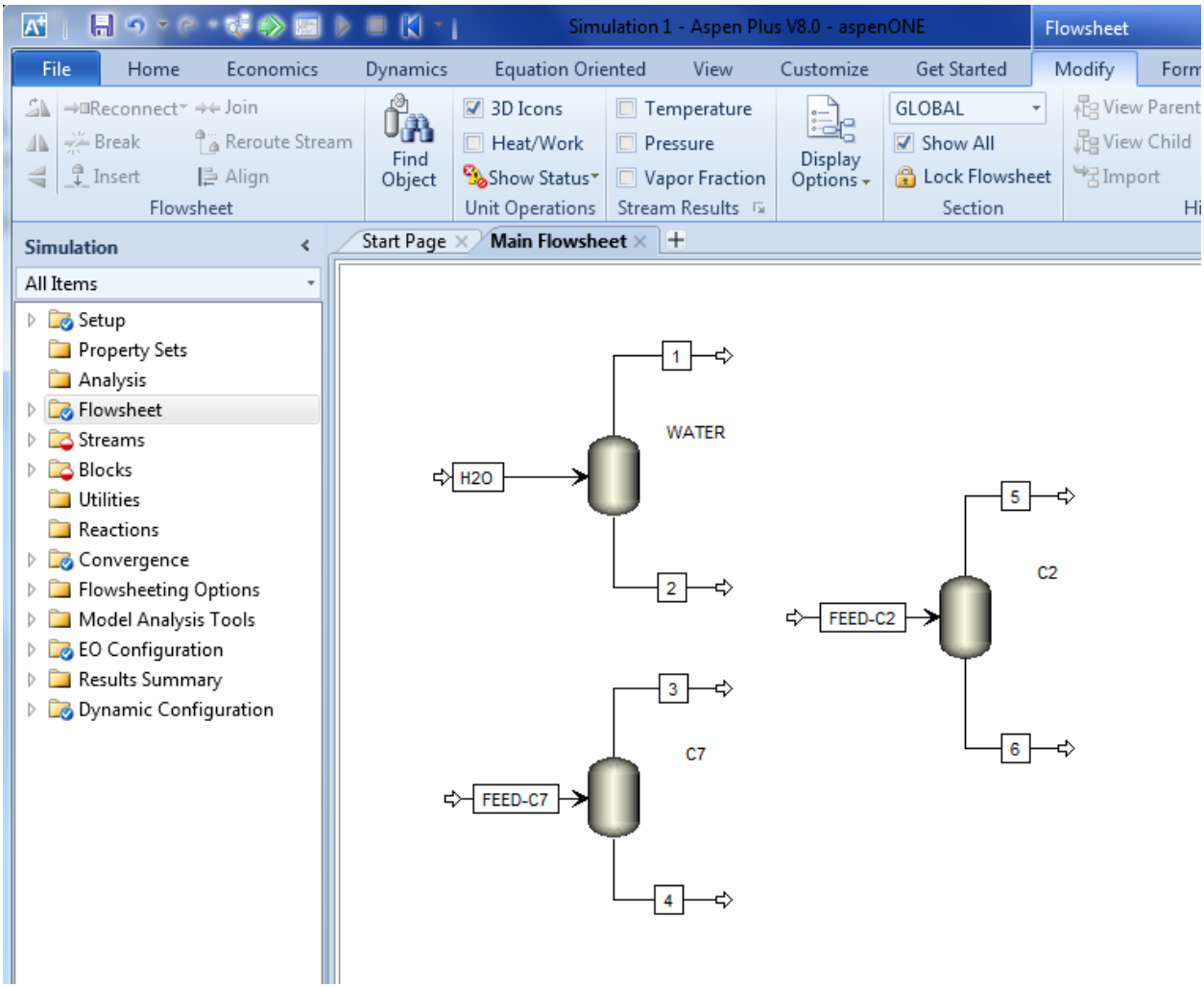
4.01. Create a new simulation in Aspen Plus using the **Blank Simulation** template. The **Components | Specification | Selection** sheet is displayed. Enter **WATER**, **C7H16-3**, and **C2H3CL3** for **Component ID**.



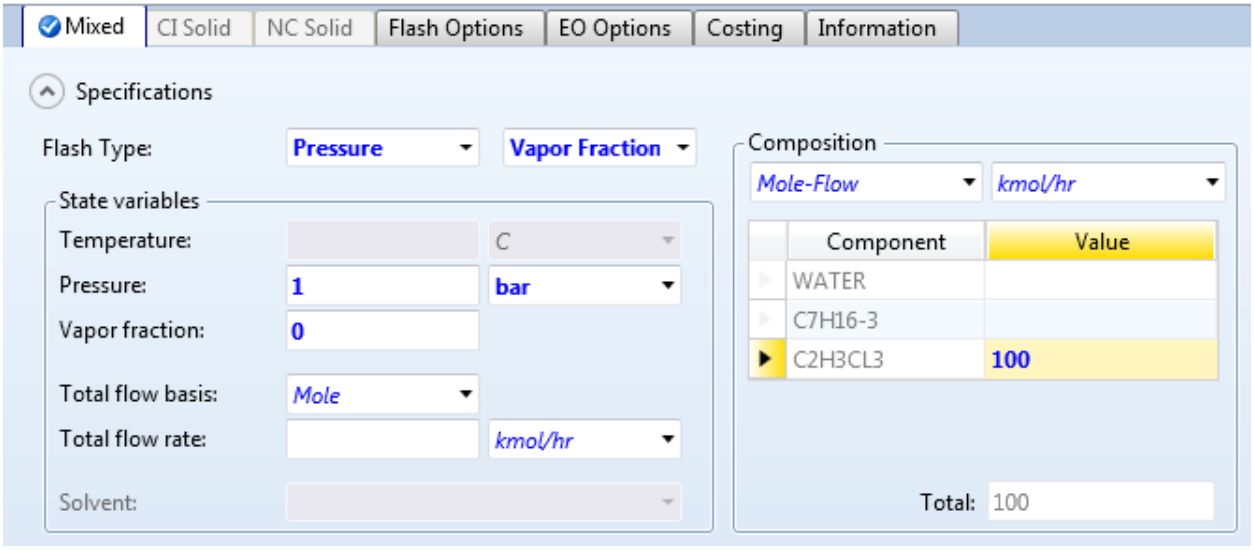
4.02. In the **Methods | Specifications | Global** sheet, select **UNIQ-RK** for **Method name**. Then, click the **Next Input** button (or press the **F4** key) to populate the binary interaction parameters.



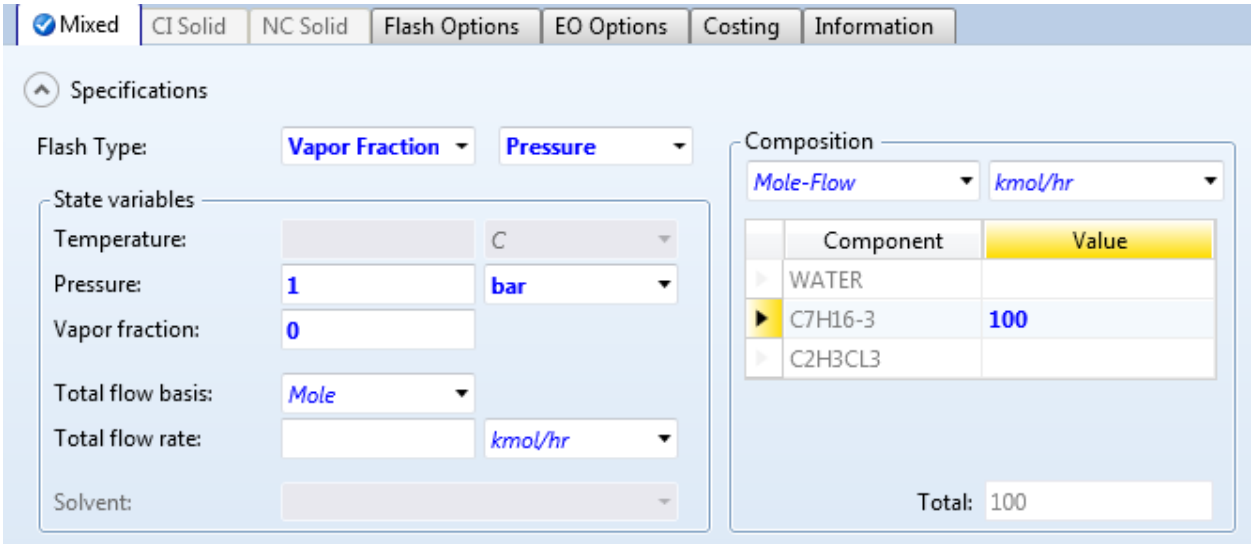
4.03. Enter the Simulation environment. Add three separate **Flash2** blocks and attach **Material Streams** accordingly. For this step, only attach streams to required ports (i.e., ports in red). Rename the streams and blocks as shown below.



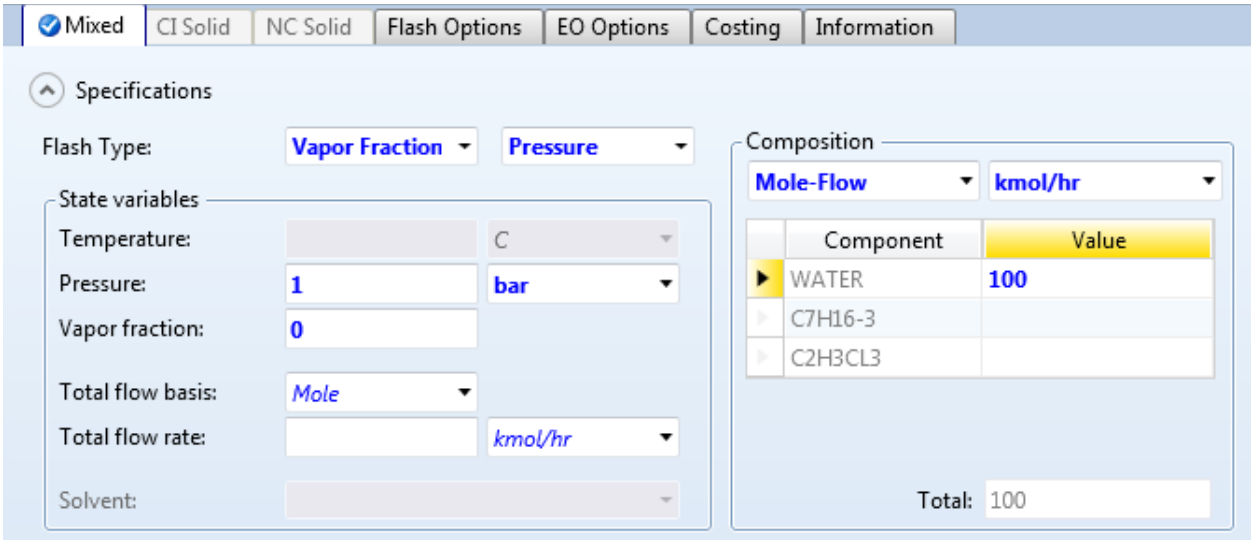
4.04. In the **Streams | FEED-C2 | Input | Mixed** sheet, select **Pressure** and **Vapor Fraction** in drop-down lists for **Flash Type**. Enter **1** for the **Pressure** value field, and **0** for the **Vapor fraction** value field. Select **bar** for the **Pressure** unit field. This sets the stream condition to that of saturated liquid at 1 bar. In the **Composition** frame, select **Mole-Flow** and **kmol/hr** from the drop-down lists and enter **100** for **C2H3CL3**.



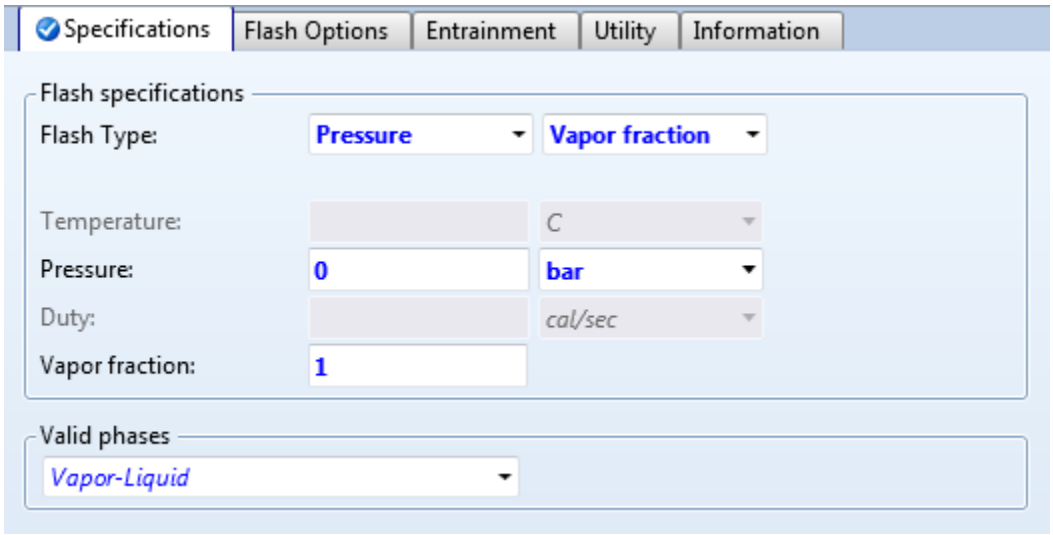

4.05. Repeat step 4.04 for stream **Feed-C7**. Enter **100** for **C7H16-3**.



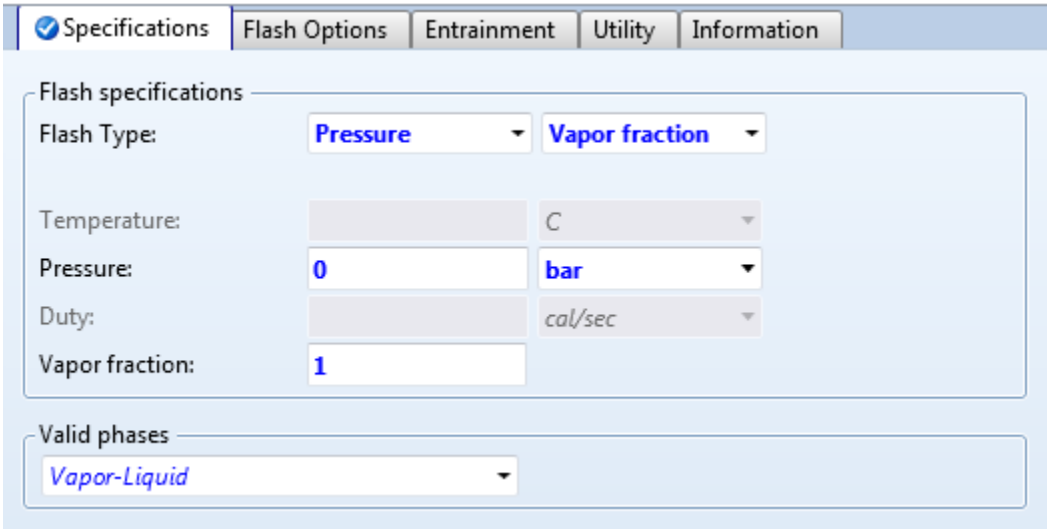
4.06. Repeat step 4.04 for stream **H2O**. Enter **100** for **WATER**.



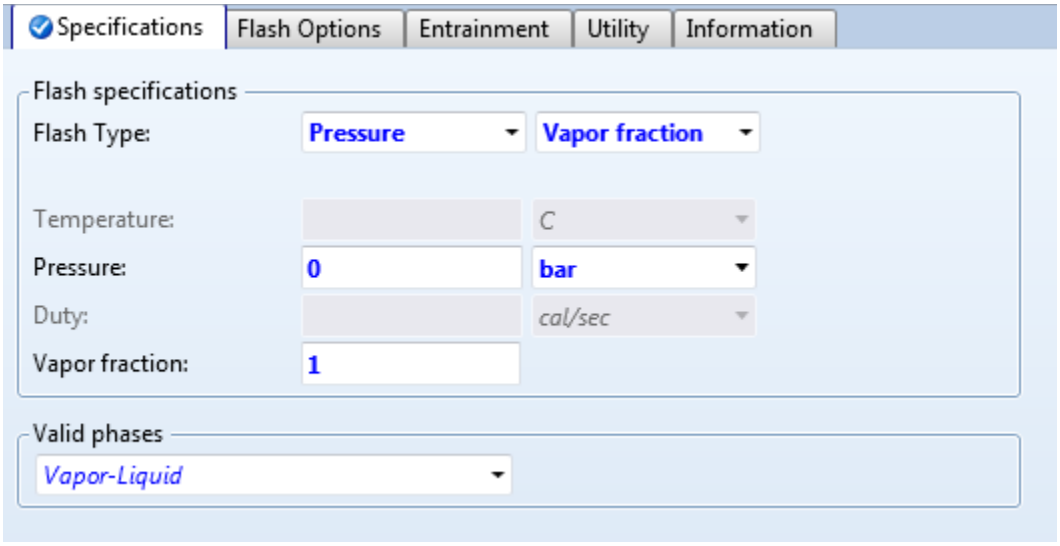

4.07. In the **Blocks | C2 | Input | Specifications** sheet, select **Pressure** and **Vapor Fraction** from drop-down lists for **Flash Type**. Enter **0** for **Pressure** and **1** for **Vapor fraction**. A pressure of **0** means no pressure drop across the flash drum. The calculated heat duty is the heat of vaporization at 1 bar for trichloroethane.



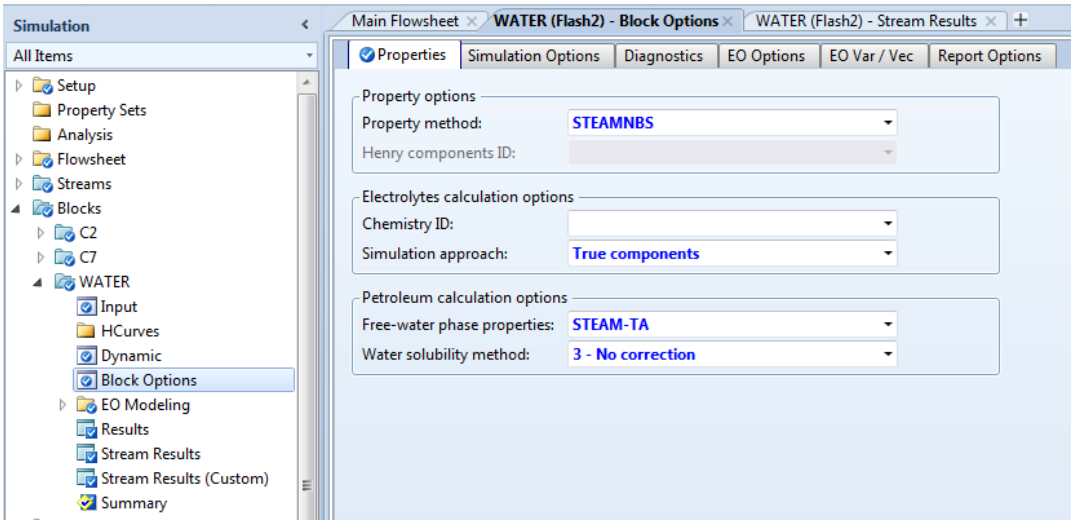
4.08. Repeat step 4.07 for block **C7** with the same specifications.



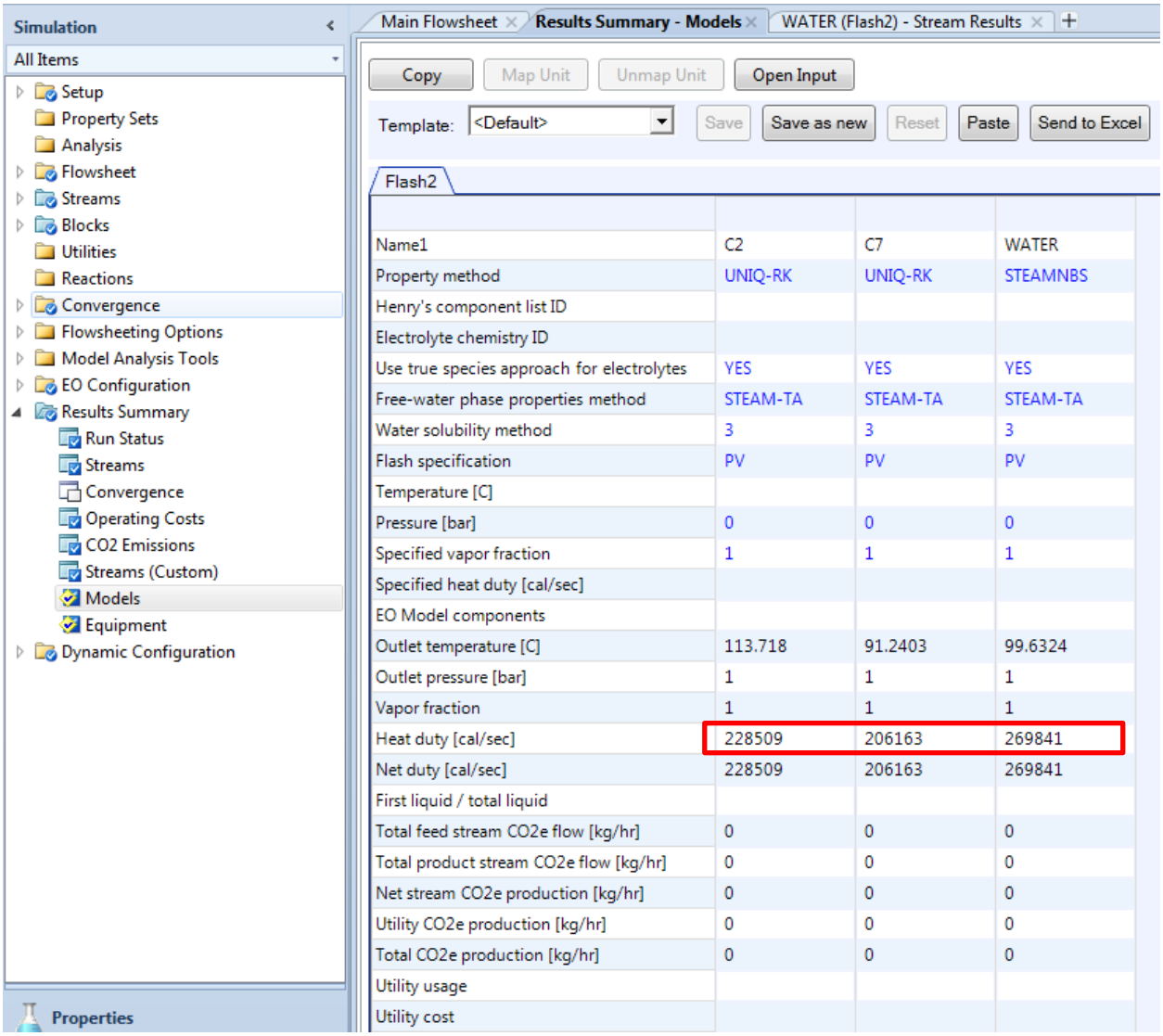

4.09. Repeat step 4.07 for block **WATER** with the same specifications.



4.10. For block **WATER** we must also change the property method to **STEAMNBS**. When using pure water with no other components, other methods can sometimes be inaccurate when it comes to density and heat capacity of water. To do this navigate to the **Blocks | WATER | Block Options** form and select **STEAMNBS** for **Property Method**.




4.11. Select the **Run** button under the **Home** tab of the ribbon (or press the **F5** key) to run the simulation. Once it is complete, the results are available on the **Results Summary | Models | Flash2** sheet. Each **Heat duty** in the red box is the amount of energy required to vaporize 100 kmol/hr of the relevant species at 1 bar. The heat of vaporization for each species can be calculated via division of the heat duty by the molar flow rate.




| | | | |
|---|---|---|---|
| Name1 | C2 | C7 | WATER |
| Property method | UNIQ-RK | UNIQ-RK | STEAMNBS |
| Henry's component list ID | | | |
| Electrolyte chemistry ID | | | |
| Use true species approach for electrolytes | YES | YES | YES |
| Free-water phase properties method | STEAM-TA | STEAM-TA | STEAM-TA |
| Water solubility method | 3 | 3 | 3 |
| Flash specification | PV | PV | PV |
| Temperature [C] | | | |
| Pressure [bar] | 0 | 0 | 0 |
| Specified vapor fraction | 1 | 1 | 1 |
| Specified heat duty [cal/sec] | | | |
| EO Model components | | | |
| Outlet temperature [C] | 113.718 | 91.2403 | 99.6324 |
| Outlet pressure [bar] | 1 | 1 | 1 |
| Vapor fraction | 1 | 1 | 1 |
| Heat duty [cal/sec] | 228509 | 206163 | 269841 |
| Net duty [cal/sec] | 228509 | 206163 | 269841 |
| First liquid / total liquid | | | |
| Total feed stream CO2e flow [kg/hr] | 0 | 0 | 0 |
| Total product stream CO2e flow [kg/hr] | 0 | 0 | 0 |
| Net stream CO2e production [kg/hr] | 0 | 0 | 0 |
| Utility CO2e production [kg/hr] | 0 | 0 | 0 |
| Total CO2e production [kg/hr] | 0 | 0 | 0 |
| Utility usage | | | |
| Utility cost | | | |

## 5. Conclusions

Although water has small molecular weight, its heat of vaporization is large. Heat of vaporization for water is about 18% higher than that of 1,1,2-trichloroethane and about 30% higher than that of 3-methylhexane.

## 6. Copyright