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.
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.
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