

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

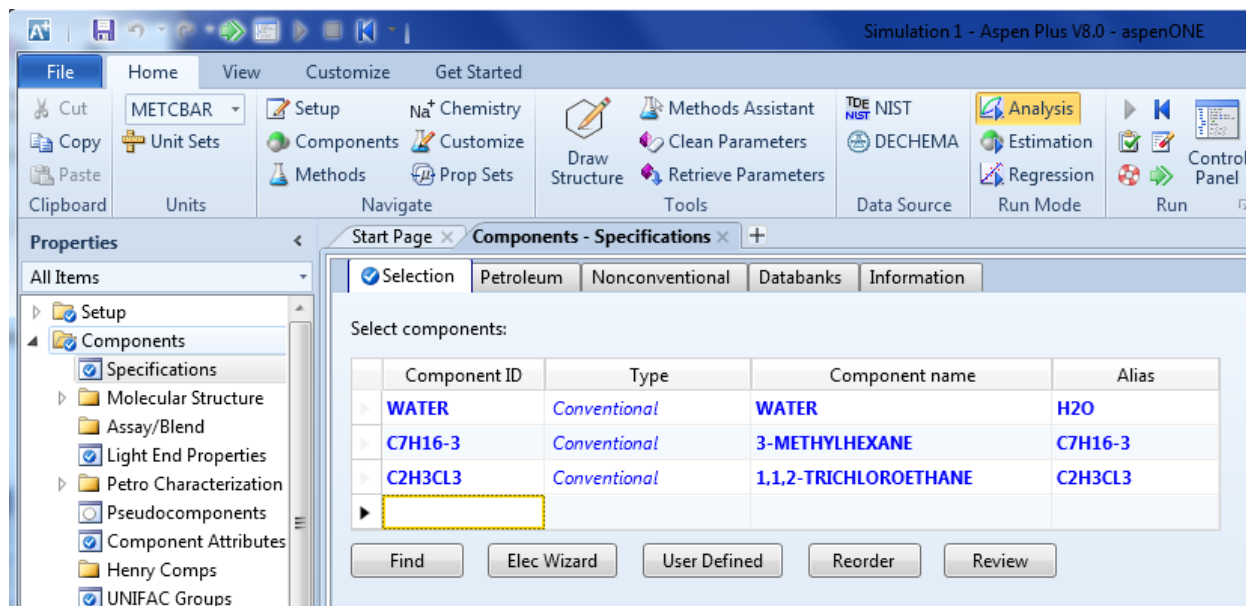
The driving force for distillation is energy. The most energy consuming part of a distillation column is the vaporization of material in the reboiler to cause vapor to flow from the bottom of the column to the top of the column. Heat of vaporization determines the amount of energy required. Therefore, 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**.

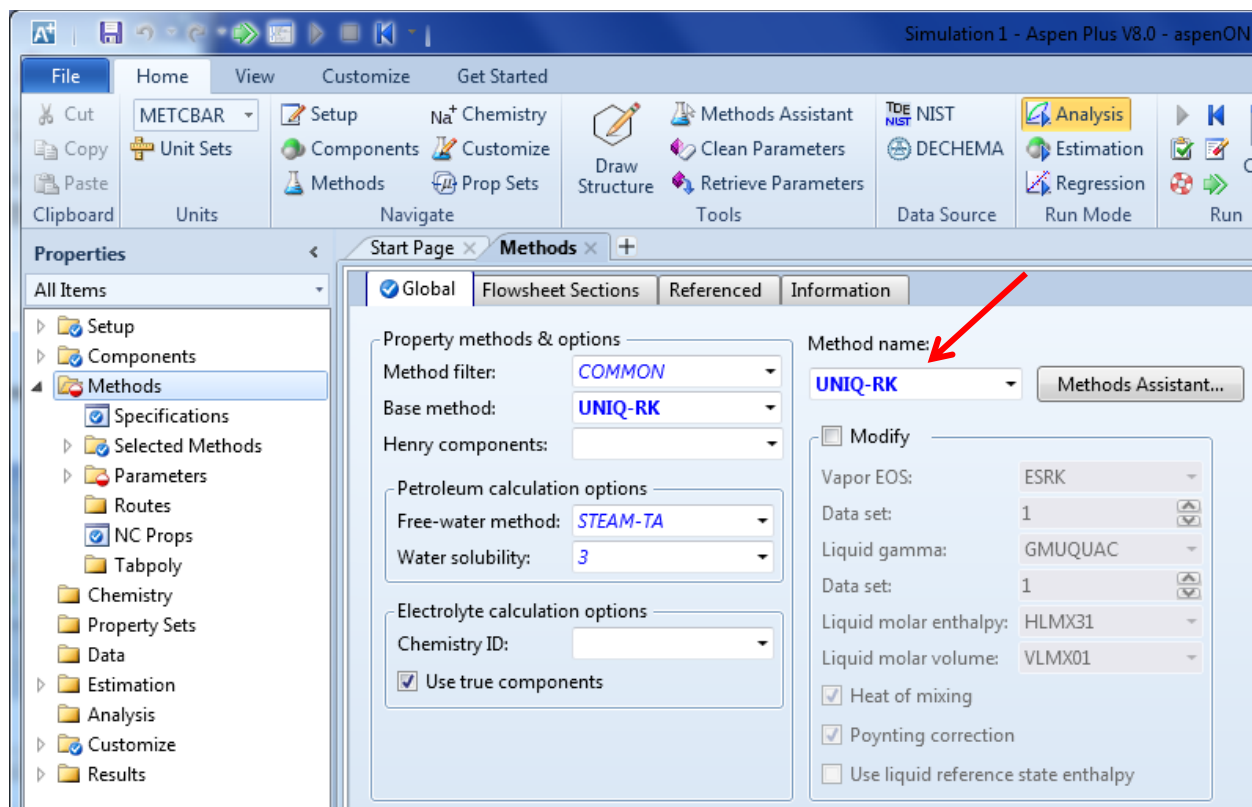


The screenshot shows the Aspen Plus V8.0 interface. The main window displays the 'Components - Specifications' sheet, specifically the 'Selection' tab. The 'Select components:' table is visible, with the following data:

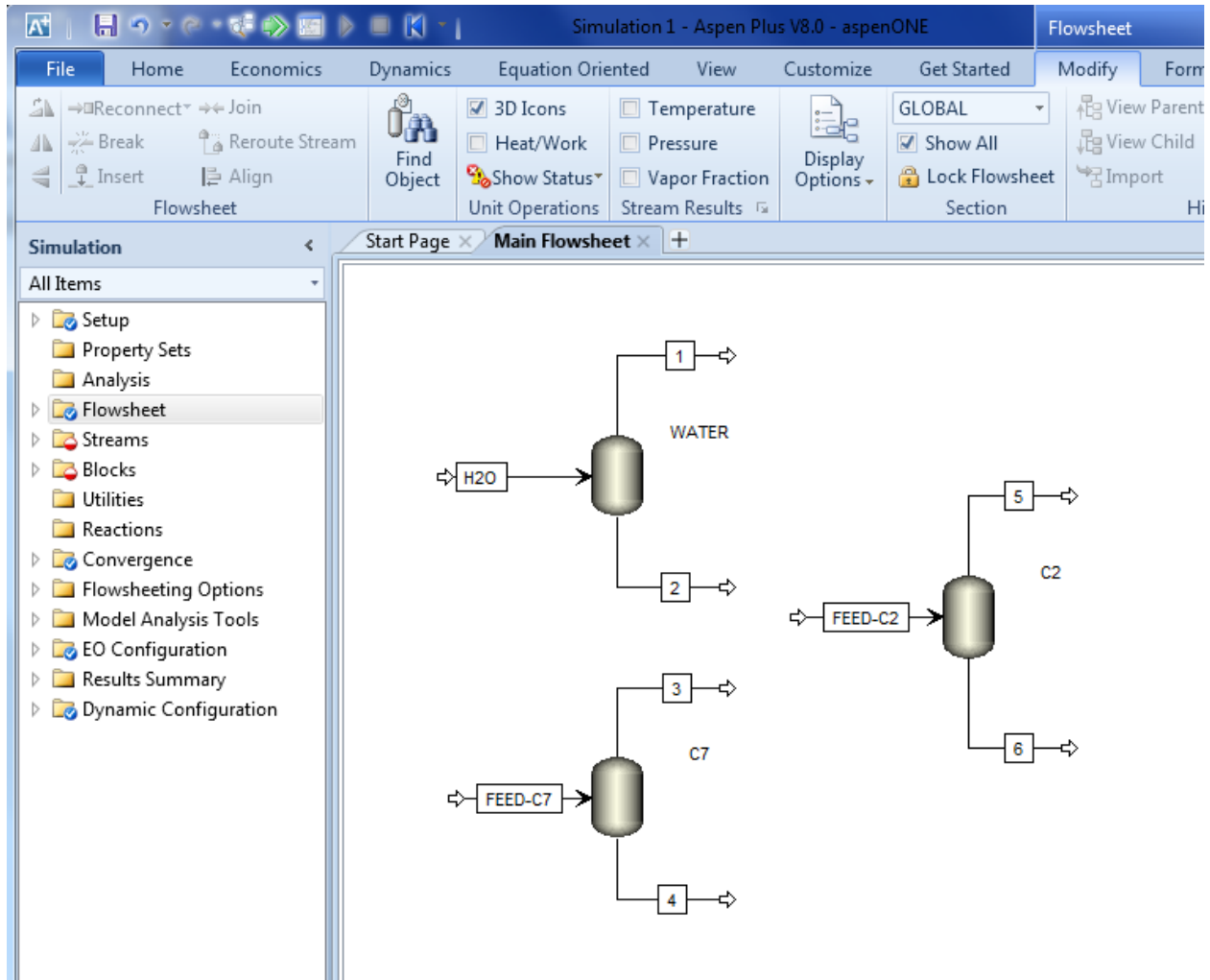
Component ID	Type	Component name	Alias
WATER	Conventional	WATER	H2O
C7H16-3	Conventional	3-METHYLHEXANE	C7H16-3
C2H3CL3	Conventional	1,1,2-TRICHLOROETHANE	C2H3CL3

Below the table are buttons for 'Find', 'Elec Wizard', 'User Defined', 'Reorder', and 'Review'. The left sidebar shows the 'Properties' pane with 'Components' expanded, and 'Specifications' selected. The top ribbon includes 'File', 'Home', 'View', 'Customize', and 'Get Started' tabs.

- 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**.

Mixed CI Solid NC Solid Flash Options EO Options Costing Information

Specifications

Flash Type: Pressure Vapor Fraction

State variables

Temperature: C

Pressure: 1 bar

Vapor fraction: 0

Total flow basis: Mole

Total flow rate: kmol/hr

Solvent:

Composition

Mole-Flow kmol/hr

Component	Value
WATER	
C7H16-3	
C2H3CL3	100

Total: 100

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

Mixed CI Solid NC Solid Flash Options EO Options Costing Information

Specifications

Flash Type: Vapor Fraction Pressure

State variables

Temperature: C

Pressure: 1 bar

Vapor fraction: 0

Total flow basis: Mole

Total flow rate: kmol/hr

Solvent:

Composition

Mole-Flow kmol/hr

Component	Value
WATER	
C7H16-3	100
C2H3CL3	

Total: 100

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

Specifications

Flash Type: **Vapor Fraction** **Pressure**

State variables

Temperature: C

Pressure: **bar**

Vapor fraction:

Total flow basis: **Mole**

Total flow rate: **kmol/hr**

Solvent:

Composition

Mole-Flow **kmol/hr**

Component	Value
▶ WATER	100
▶ C7H16-3	
▶ C2H3CL3	

Total:

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.

Specifications

Flash specifications

Flash Type: **Pressure** **Vapor fraction**

Temperature: C

Pressure: **bar**

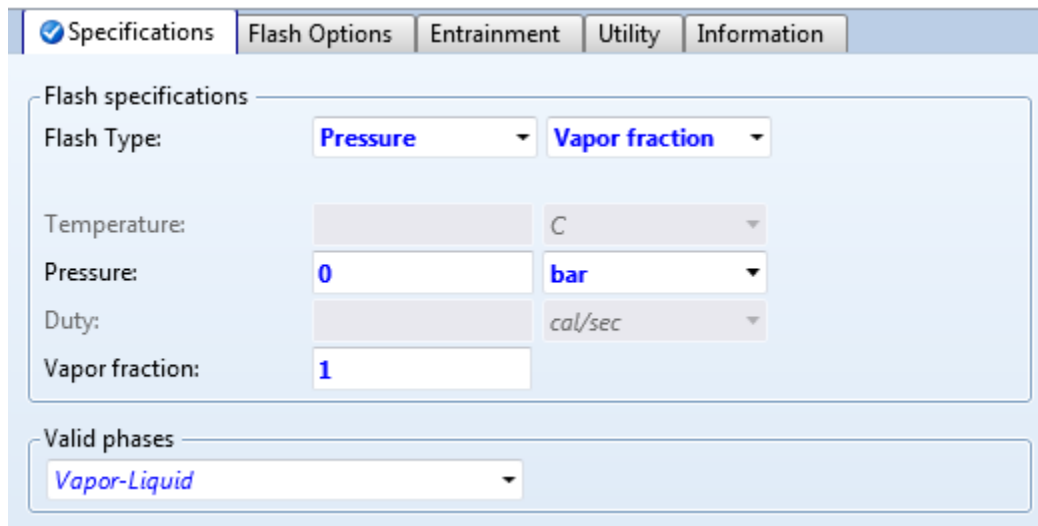
Duty: **cal/sec**

Vapor fraction:

Valid phases

Vapor-Liquid

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

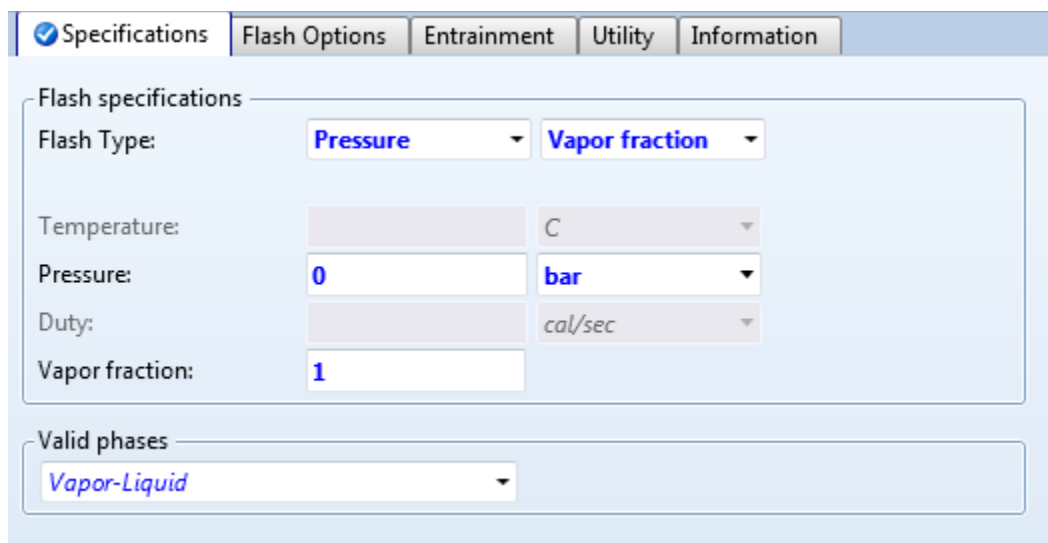


The screenshot shows the 'Specifications' tab for block C7. The 'Flash specifications' section includes the following fields:

- Flash Type: Pressure (dropdown)
- Vapor fraction: Vapor fraction (dropdown)
- Temperature: (empty text box) C (dropdown)
- Pressure: 0 (text box) bar (dropdown)
- Duty: (empty text box) cal/sec (dropdown)
- Vapor fraction: 1 (text box)

The 'Valid phases' section shows a dropdown menu with 'Vapor-Liquid' selected.

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

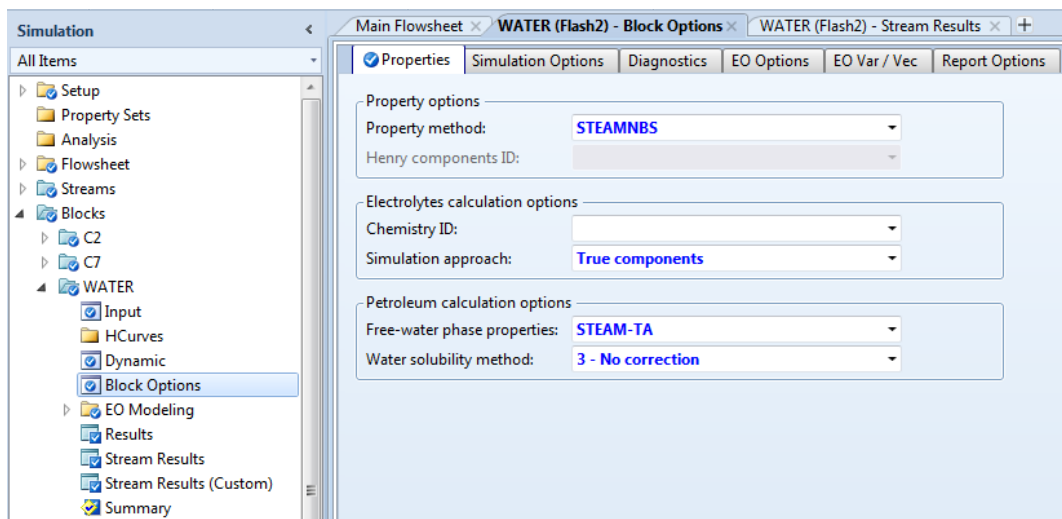


The screenshot shows the 'Specifications' tab for block WATER. The 'Flash specifications' section includes the following fields:

- Flash Type: Pressure (dropdown)
- Vapor fraction: Vapor fraction (dropdown)
- Temperature: (empty text box) C (dropdown)
- Pressure: 0 (text box) bar (dropdown)
- Duty: (empty text box) cal/sec (dropdown)
- Vapor fraction: 1 (text box)

The 'Valid phases' section shows a dropdown menu with 'Vapor-Liquid' selected.

- 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.

Simulation < Main Flowsheet x Results Summary - Models x WATER (Flash2) - Stream Results x +

Copy Map Unit Unmap Unit Open Input

Template: <Default> Save Save as new Reset Paste Send to Excel

Flash2

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			

Properties

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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