What's New in *ChemSep*™ 8.00 – 8.11

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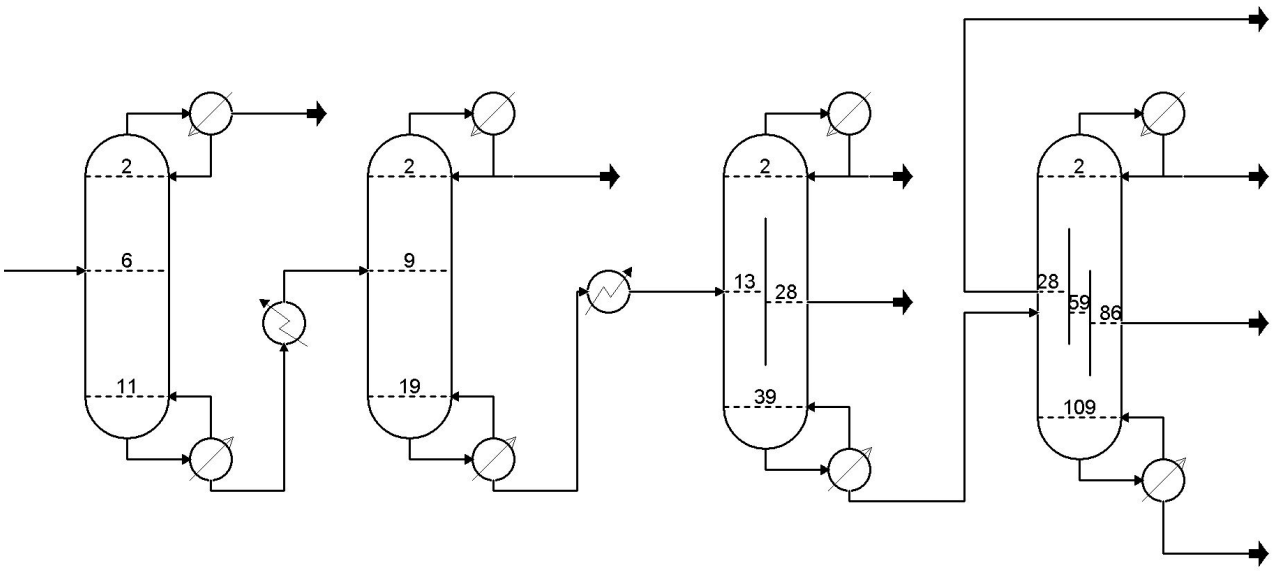
In this document we discuss the new and improved features in ***ChemSep***:

1. **New: Dividing Wall Columns**
2. **New: Stream Curves**
3. **New: Aids to Converging Difficult Cases**
4. **Extrapolation of ideal gas heat capacity to high temperatures**
5. **Loading of large problem files**
6. **Miscellaneous Updates**

The illustration below shows the final separation train of a process in which the last two columns are using the new ChemSep model for Dividing Wall Columns (DWCs). We used the COFE (CAPE-OPEN Flowsheeting Environment) to make this flowsheet in part because COFE is freely available, but also because COFE is the only CAPE-OPEN flowsheet simulation package with adaptable unit operation icons. In other words, a ChemSep DWC column inserted into a COFE flowsheet looks like a DWC. A ChemSep column inserted into another package will be displayed using a standard icon that that package uses for all CAPE-OPEN unit operations. The original process was separating a mixture of nineteen components using 7 columns. In the revised process shown below two DWCs replace 5 ordinary columns.

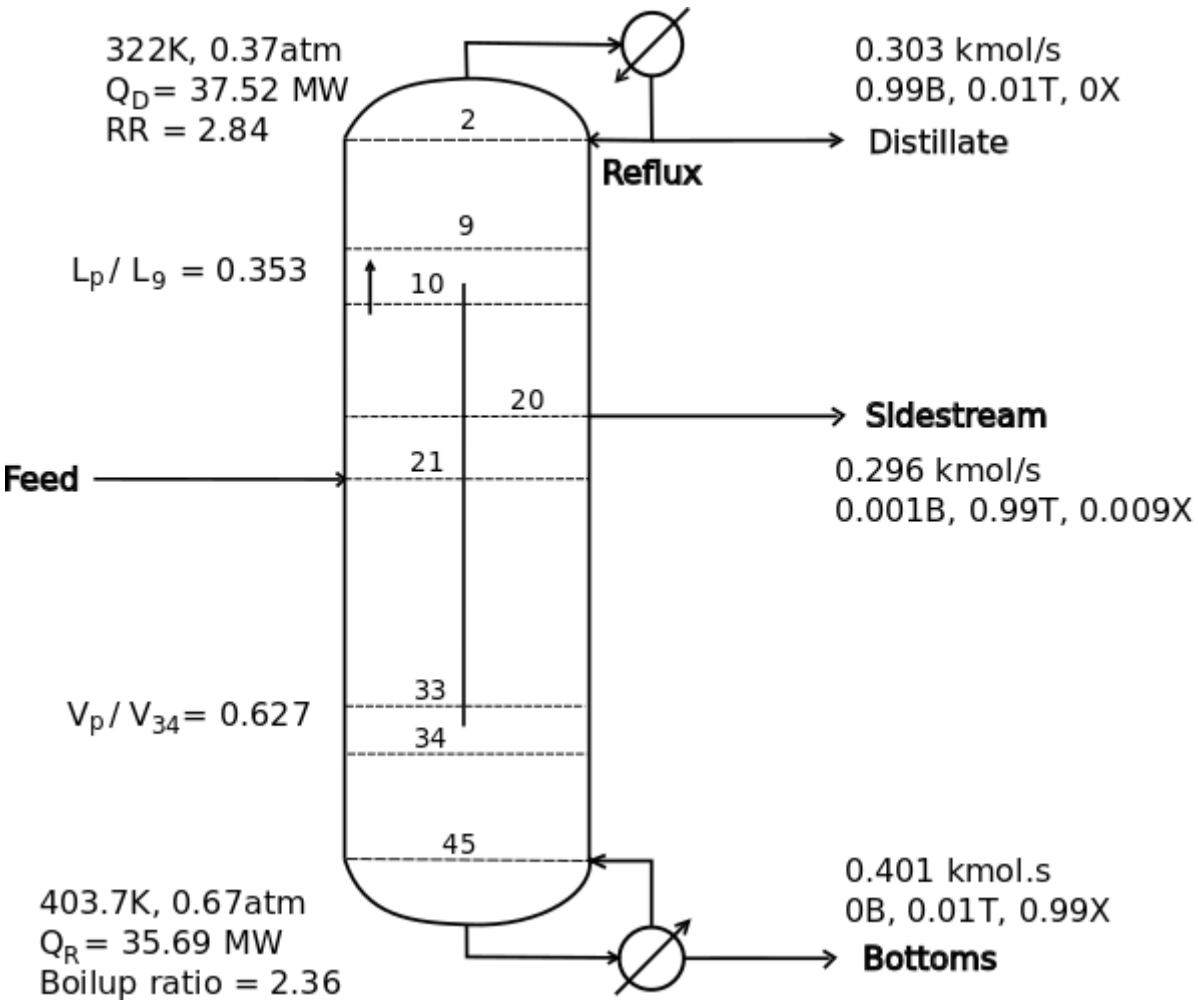


New: Dividing Wall Columns

Dividing wall columns (DWC) have attracted considerable attention in recent years. It is often stated that no commercial flowsheet simulation package has yet offered a DWC as a standard model. As a result, nearly all simulations of DWCs employ interlinked multi-column equilibrium stage models in a sequential-modular process simulator. It is claimed that equation-based simulators offer advantages over sequential modular simulators when modelling DWCs but, to date, no empirical evidence in support of such a contention has been published.

In version 8.0 we added the ability to simulate dividing wall columns in ChemSep (equilibrium stage models only so far). The technical details of what we call a Parallel Column Model (PCM) are described by Zhou et al. (Computers and Chemical Engineering, Under Review, 2018). Only a brief illustration can be given here.

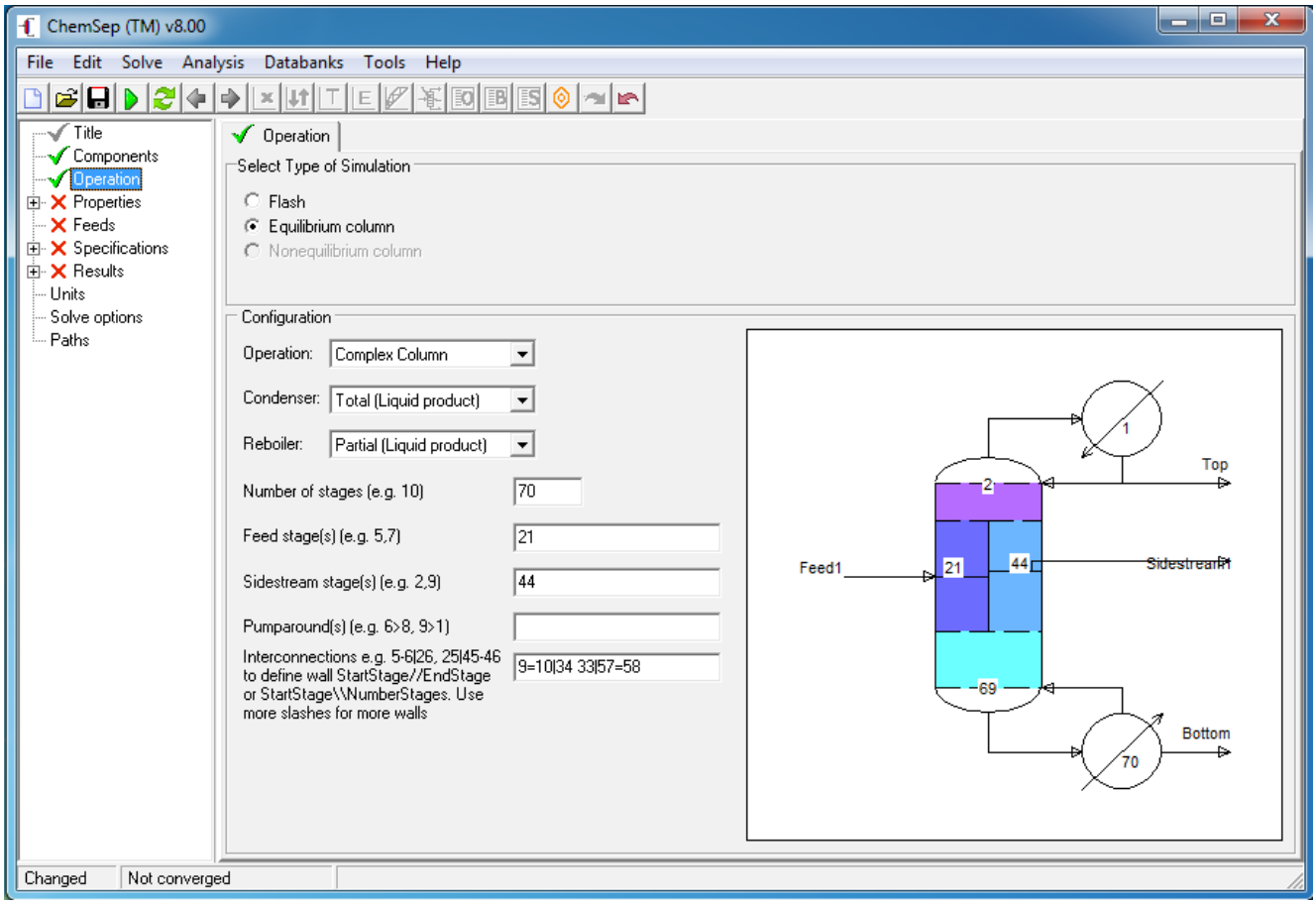
The schematic diagram shown below shows a dividing wall column for separation of this ternary system, with additional information about the simulation. This diagram is adapted from Figure 12.1 in Luyben (2013). L_p and V_p in the figure below represent the liquid and vapor flowrates going to the pre-fractionator (or left side of the wall). In this work, the liquid (or vapor) split ratio is defined to be the liquid (or vapor) flowrate going to the left side of the wall divided by the total amount of liquid (or vapor) flowing down (or up).



Before starting ChemSep, the first thing we should work out is the column stage numbering. This is an important step when creating an equation-oriented model. Based on the figure above, this column has 9 stages in the top section (the condenser is treated as a stage), 24 stages in each section beside the dividing

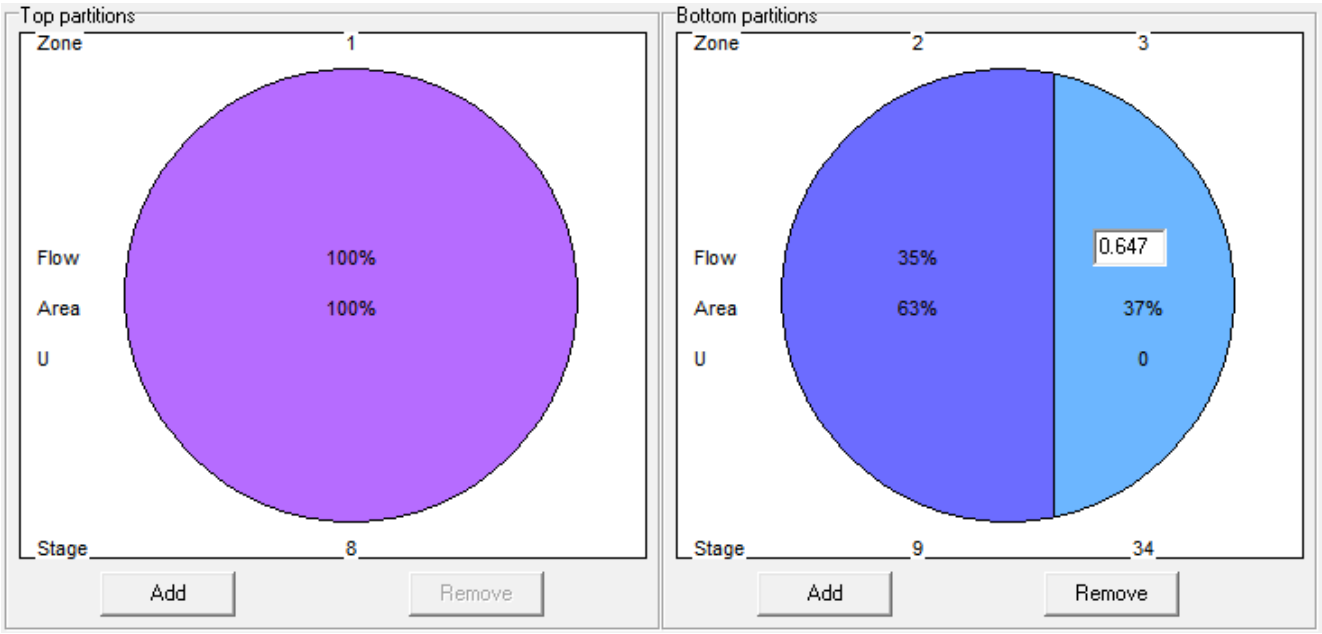
wall, and 13 stages in the bottom section (the reboiler is treated as another stage). In ChemSep stages are numbered from the top with the condenser and reboiler both included in the numbering; thus, the condenser is stage 1. The total number of stages in this DWC model is, therefore, 70. We then number all the stages in this column in the following order: top -> left -> right -> bottom, and work out the corresponding feed and side stream stages. The resulting column stage numbers in the Parallel Column Model (PCM) is shown in the figure above. For more information on numbering stages in the PCM refer to Zhou et al. (2018).

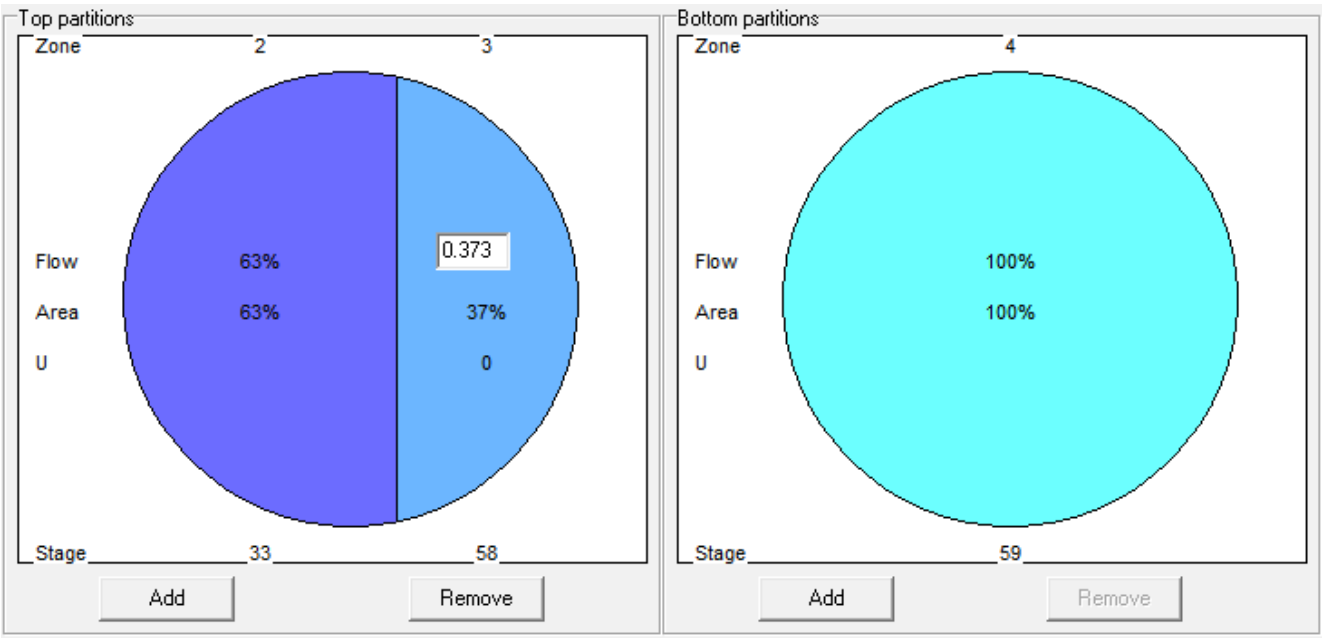
The configuration of a DWC is done on the *Operation* panel in ChemSep. The image below shows the DWC under discussion.



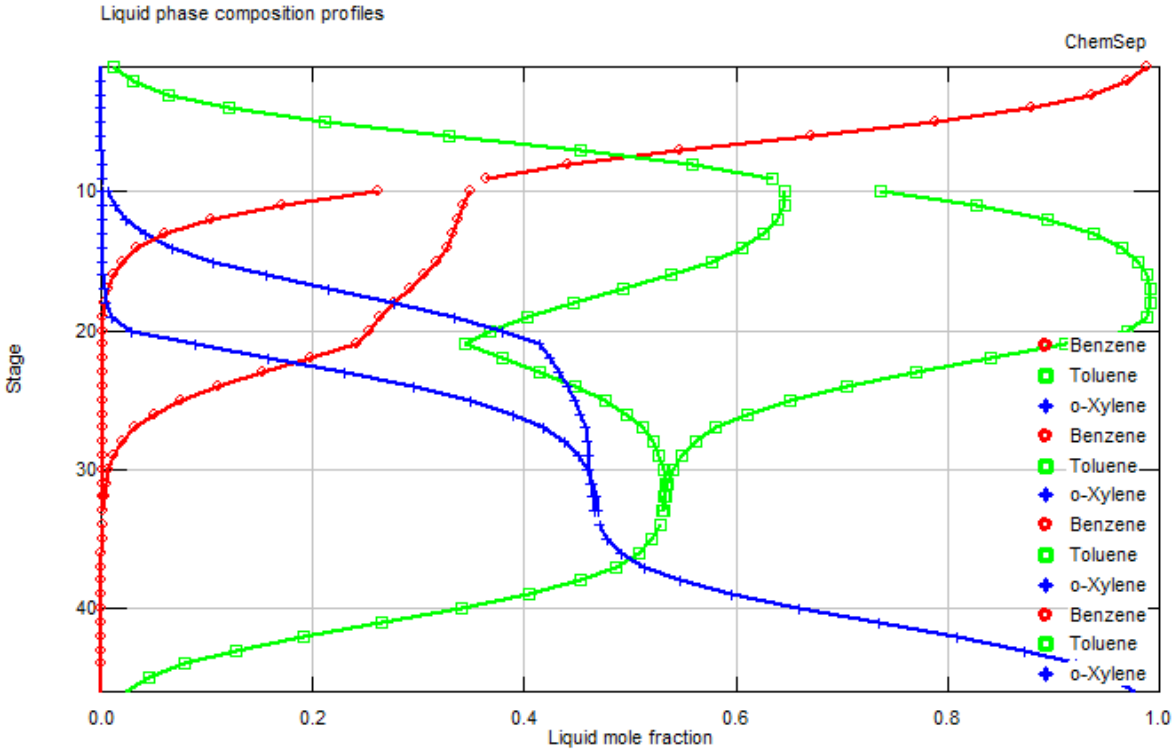
This action will create a new *Interconnections* panel to become visible. This is where we specify the vapor and liquid flow splits.

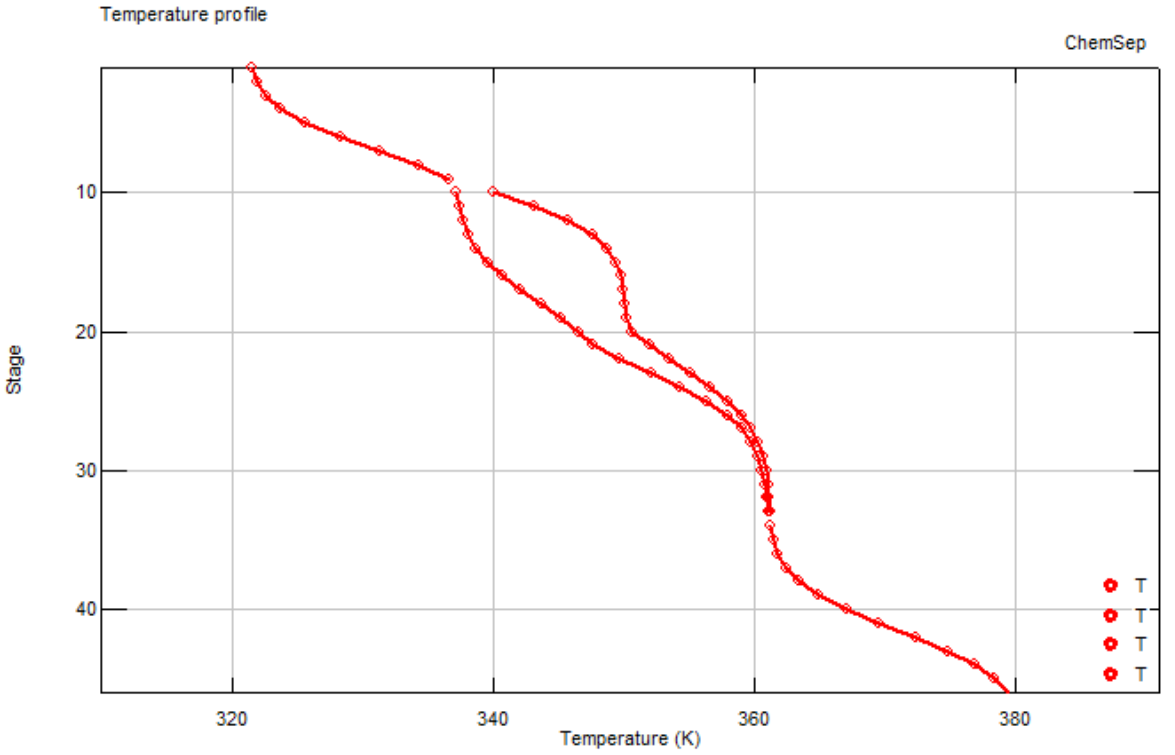
On the Interconnections tab, users can specify the vapor and liquid split ratios of a dividing wall. The liquid split ratio is provided as 0.353, meaning 35.3% of the liquid on stage 9 flows to stage 10, while 64.7% flows to stage 34. Applying similar reasoning, we specify the vapor split ratio at the bottom of the wall to be 62.7% / 37.3%. Note that the dividing wall is not located right at the middle of the cross-sectional area of the column, and this can be realized by specifying the Area ratios on two sides of the wall. Here we use the ratio of the vapor flows to approximate the ratio of the cross-sectional area on two sides of the wall. Specifications of the interconnections are shown in the screenshots below:


Top partitions
Zone
1
Flow
100%
Area
100%
U
Stage
8
Add
Remove
Bottom partitions
Zone
2
3
Flow
35%
0.647
Area
63%
37%
U
0
Stage
9
34
Add
Remove


Top partitions
Zone
2
3
Flow
63%
0.373
Area
63%
37%
U
0
Stage
33
58
Add
Remove
Bottom partitions
Zone
4
Flow
100%
Area
100%
U
Stage
59
Add
Remove

The completion of a DWC model is much the same as any other column. Display of results shows some interesting aspects of DWCs:



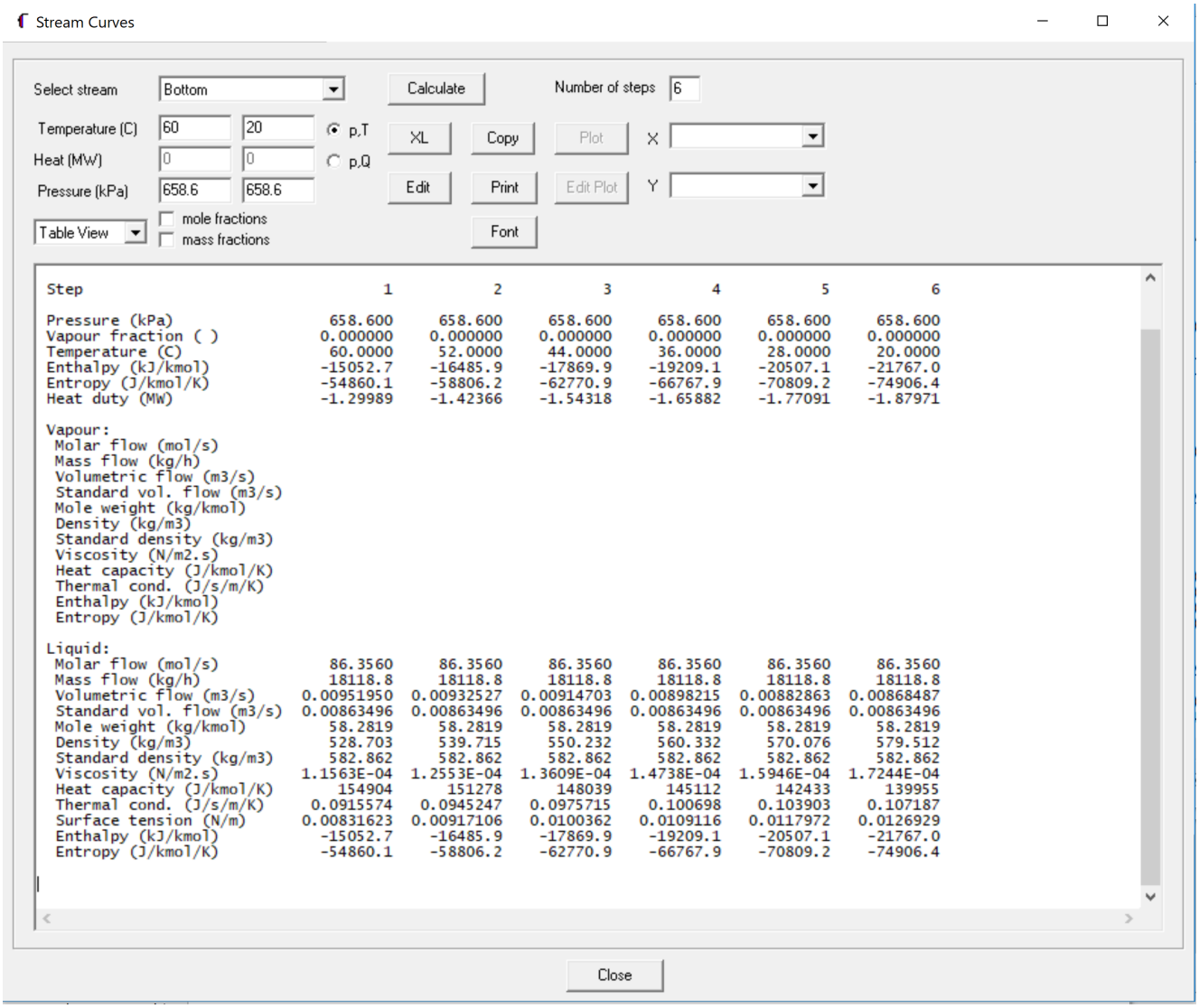


At present ChemSep includes only an equiibrium stage model for DWCs. Rate-bsed models will be available later in 2019.

New: Stream Curves

We have added the *Stream Curves* tool that allow calculation of heating/cooling curves for heat exchanger design or deeper analysis. Any product stream or internal stream can be selected, and any combination of pressure and temperature or heat duty increase / decrease can be applied, as to facilitate the generation of stream curves for condensers and reboilers.

Stream curves can be found in the *Analysis* menu.



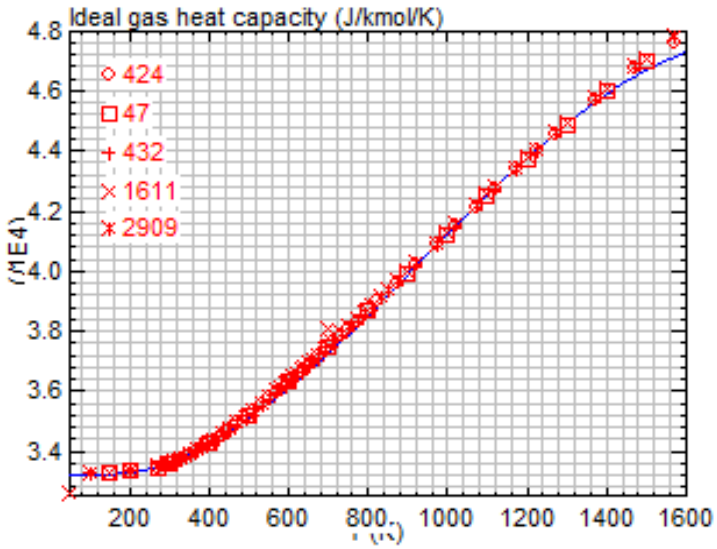
Step	1	2	3	4	5	6
Pressure (kPa)	658.600	658.600	658.600	658.600	658.600	658.600
Vapour fraction ( )	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Temperature (C)	60.0000	52.0000	44.0000	36.0000	28.0000	20.0000
Enthalpy (kJ/kmol)	-15052.7	-16485.9	-17869.9	-19209.1	-20507.1	-21767.0
Entropy (J/kmol/K)	-54860.1	-58806.2	-62770.9	-66767.9	-70809.2	-74906.4
Heat duty (MW)	-1.29989	-1.42366	-1.54318	-1.65882	-1.77091	-1.87971
Vapour:						
Molar flow (mol/s)						
Mass flow (kg/h)						
Volumetric flow (m3/s)						
Standard vol. flow (m3/s)						
Mole weight (kg/kmol)						
Density (kg/m3)						
Standard density (kg/m3)						
Viscosity (N/m2.s)						
Heat capacity (J/kmol/K)						
Thermal cond. (J/s/m/K)						
Enthalpy (kJ/kmol)						
Entropy (J/kmol/K)						
Liquid:						
Molar flow (mol/s)	86.3560	86.3560	86.3560	86.3560	86.3560	86.3560
Mass flow (kg/h)	18118.8	18118.8	18118.8	18118.8	18118.8	18118.8
Volumetric flow (m3/s)	0.00951950	0.00932527	0.00914703	0.00898215	0.00882863	0.00868487
Standard vol. flow (m3/s)	0.00863496	0.00863496	0.00863496	0.00863496	0.00863496	0.00863496
Mole weight (kg/kmol)	58.2819	58.2819	58.2819	58.2819	58.2819	58.2819
Density (kg/m3)	528.703	539.715	550.232	560.332	570.076	579.512
Standard density (kg/m3)	582.862	582.862	582.862	582.862	582.862	582.862
Viscosity (N/m2.s)	1.1563E-04	1.2553E-04	1.3609E-04	1.4738E-04	1.5946E-04	1.7244E-04
Heat capacity (J/kmol/K)	154904	151278	148039	145112	142433	139955
Thermal cond. (J/s/m/K)	0.0915574	0.0945247	0.0975715	0.100698	0.103903	0.107187
Surface tension (N/m)	0.00831623	0.00917106	0.0100362	0.0109116	0.0117972	0.0126929
Enthalpy (kJ/kmol)	-15052.7	-16485.9	-17869.9	-19209.1	-20507.1	-21767.0
Entropy (J/kmol/K)	-54860.1	-58806.2	-62770.9	-66767.9	-70809.2	-74906.4

Display of mole and/or mass fraction is optional but you have to click on calculate again to see them.

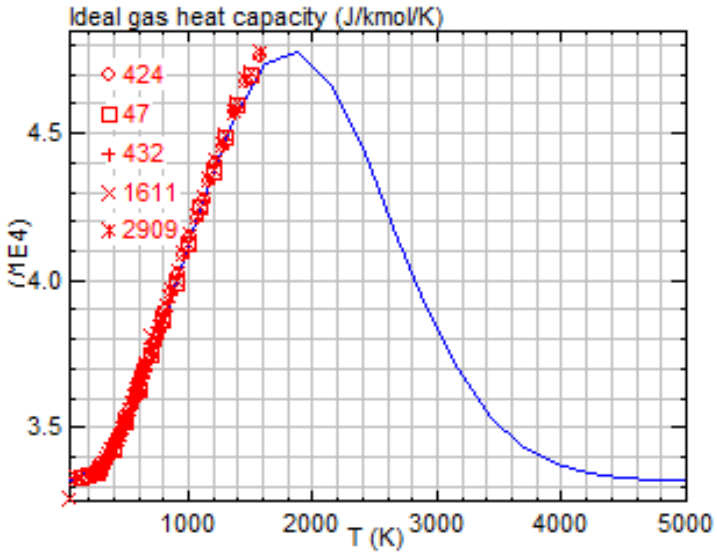
Extrapolation of CpIG to High Temperatures

An essential part of the calculation of enthalpy is the integration of the ideal gas heat capacity over the range from the reference temperature to the temperature of the stream. For most compounds in ChemSep the ideal gas heat capacity correlations are fit to data in the range up 1000 K or 1500 K.

Here, for example, is water.



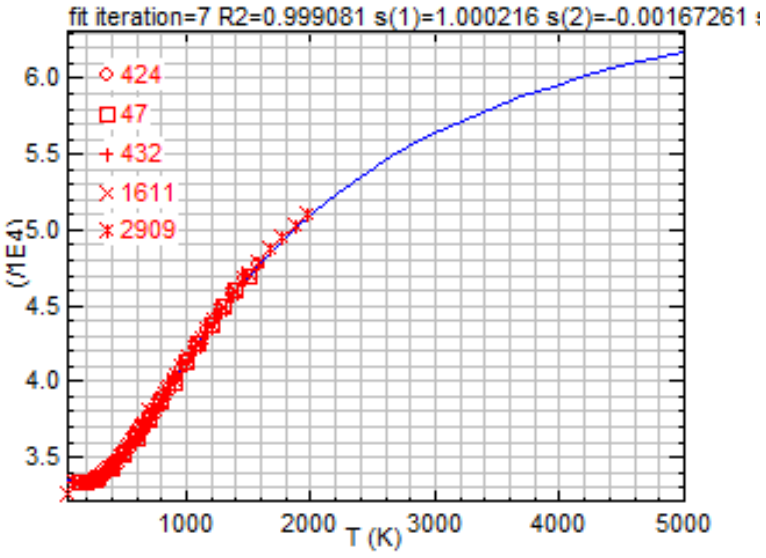
On occasion, however, it is necessary to evaluate the heat capacity at temperatures outside the valid range of the ChemSep correlations. Here is what happens if we extrapolate that correlation to 5000K.



Clearly, not a correct extrapolation. (We should note that this is very far beyond the range at which any two-phase separation would be possible, so at these high temperatures we are dealing only with gas phases. That said, it remains possible that in a process flowsheet it might be necessary to evaluate the ideal gas heat capacity at temperatures outside the valid range.

We added a new type of extrapolation for CpIG to very high temperatures e.g. 10000 K. The new extrapolation is based on the method of Bruel, Chiron, Tavares, and Patience, *An Exponential Expression for Gas Heat*

Capacity, Enthalpy, and Entropy, Experimental Thermal and Fluid Science 78 (November 2016): 249–53 (https://doi.org/10.1016/j.expthermflusci.2016.06.008). For water the extrapolation looks like this:



The parameters for the new extrapolation are computed for every compound at the start of the simulation and are used ONLY when it is necessary to evaluate the ideal gas heat capacity at a temperature outside the valid range. That is, for temperatures in the valid range of the ChemSep correlation the existing correlation will still be used.

Improved Speed of Loading Large Problems

The speed of loading files for mixtures with large numbers of compounds has been improved.

New Convergence Aids in ChemSep 8.11

Version 8.11 introduces some new aids to converging what might otherwise be very difficult simulations. These include:

1. A more accurate set of “old results.”
2. An alternative method of handling non-standard specifications
3. Continuation on some non-standard specifications

These topics are discussed in detail in the *ChemSep Technical Note: Tips on Effective Problem Solving* available at www.chemsep/com/….

Miscellaneous Updates

Version 8.11 includes many small improvements such as:

- Ability to import the calculated table values from a temperature correlation, such that it can be used to fit with a different type of temperature correlation
- Ability to fit of Matthias-Copeman EOS parameters
- New molecular weight, critical temperature, critical pressure models for pseudo-compounds

Availability: As always, *ChemSep* Lite is available free from **http://chemsep.com**.