Effect of Thermodynamic Models on Separation of Aromatic Compounds

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Background:

Thermodynamic behavior of components is an integral part of design of a separation process. For instance, design and operation of distillation column primarily depends on how accurately the phase equilibrium of the components of the solution is estimated. A process engineer should assess whether the given mixture containing components behave ideally or is non-ideal. If the system is found to be non-ideal, then one has to choose appropriate thermodynamic model to estimate the phase equilibrium data. In this work a simple distillation process was simulated with two different thermodynamic models, namely Raoult's Law (ideal system) and Peng-Robinson (PR) model (one of the non-ideal models) to illustrate that thermodynamic models play a significant role in distillation column design.

Description of Flow Sheet:

A feed containing equimolar mixture of benzene and chloroform was fed to a shortcut distillation column at 25°C. Chloroform was obtained as distillate and Benzene was obtained as the bottom product. Finally, the products were cooled to room temperature. Two separate sequences of the flow sheet were developed, such that in one case, ideal Raoult's law was employed and, in another case, Peng-Robinson model was employed.

I: - Thermodynamic model

Since extractive distillation processes are strongly affected by the non-ideal interactions between the entrainer and the stream of interest, one of the main difficulties when simulating these processes is the correct thermodynamic representation of the mixture behavior in contact with the solvent. Thus, most of the work was devoted to the thermodynamic modeling.

Result:

The process flow sheet was simulated for the separation of benzene and chloroform using “shortcut column” in OpenModelica. A shortcut distillation column was simulated to calculate the actual number of stages, minimum number of stages, location of feed stage and minimum reflux ratio for the given light key and heavy key components. In the shortcut distillation column, Chloroform was taken as the light key component and Benzene as the heavy key. The light key composition at the bottoms was fixed at 0.01 and the heavy key composition at the distillate was fixed at 0.01 and a reflux ratio of 5 was assumed for the shortcut column. The shortcut column was simulated and a minimum reflux ratio of 1.76 was obtained with actual number of stages equal to 17. This process flow sheet was simulated under the property package “Raoult’s Law”.

Similarly, another flow sheet sequence for the separation of Benzene and Chloroform was simulated under the property package “Peng-Robinson (PR)”. The results obtained from the shortcut distillation column were used to specify the input parameters required for the simulation of rigorous distillation column. The rigorous column used for simulation under “Raoult’s Law” was operated at a condenser pressure of 1.01325 bar and at a reboiler pressure of 1.01325 bar. The reflux ratio was assumed to be 5.75. Similarly, the distillation column used for the simulation of the flow sheet under the property package “Peng – Robinson (PR)” was operated at a condenser and reboiler pressure of 1.01325 bar and 1.01325 bar respectively. A reflux ratio of 5 was specified and number of stages equal to 21.

Conclusions:

This study also shows that choice of thermodynamic property package has a profound effect on the design of distillation column. Open source process simulator can be used as a learning tool to assess different scenarios as illustrated in this work.

Unit System:

Temperature - °C
Pressure - bar
Molar Flow Rate – kmole/h
Mass Flow Rate – kg/h
Volumetric Flow Rate – m3/h
Density – kg/m3