Effect of Thermodynamic Models on Separation of Aromatic Compounds using Distillation Column

S. Aakash Subramanian and P. R. Naren*

School of Chemical and Biotechnology, SASTRA Deemed University

E-mail: akashsubramanian@live.com, prnaren@scbt.sastra.edu*

A. 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.

B. Description of Flow Sheet

A feed containing equi-molar 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 was developed, such that in one case, ideal Raoult's law was employed and in another case, Peng-Robinson model was employed.

C. Results

The process flow sheet was simulated for the separation of benzene and chloroform using "shortcut column" in DWSIM. 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.

From the simulated results, it can be clearly seen that choice of thermodynamic model plays a significant role in the design of the distillation column under same conditions. Without proper knowledge of the suitability of the thermodynamic model for a specific process, the probability of making errors with respect to the economic calculations of the process and the safety factor involved herein is quite high. Hence, determination of a thermodynamic model that can be applied to a process suitably takes predominance over all other factors.

Results			
Object	Distillation Column-A	Distillation Column-B	
Condenser Pressure	1.01325	1.01325	bar
Reboiler Pressure	1.01325	1.01325	bar
Reflux Ratio	5.747956	4.9982226	
Number of Stages	17	21	

D. 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: (Custom 5 in DWSIM)

Temperature - °C

Pressure - bar

Molar Flow Rate – kmol/h

Mass Flow Rate – kg/h

Volumetric Flow Rate – m^3/h

Density – kg/m^3

Reference

1. Claudia Gutiérrez-Antonio, Gustavo A. Iglesias-Silva and Arturo Jiménez-Gutiérrez, Effect of Different Thermodynamic Models on the Design of Homogeneous Azeotropic Distillation Columns. Chemical Engineering Communications, 2008, 195:9, 1059-1075