Conventional Extractive Distillation of Acetonitrile-Water Mixture

Mohik Modi and Mehulkumar Sutariya
Sardar Vallabhbhai National Institute of Technology,Surat
(modim34@gmail.com, mehulsutariya09@gmail.com)

Introduction

The chemical acetonitrile is being separated conventionally from acetonitrile-water mixture using ethylene glycol as an entrainer. High purity of acetonitrile is essential since it is used in performing High Performance Liquid Chromatography (HPLC). So separation of acetonitrile and the optimum conditions in distillation are studied from the literature [1]. Here, we have tried to simulate the proposed flowsheet with DWSIM.

Development of Flowsheet in DWSIM

All the specifications of the unit operations and thermodynamics are elaborated in the literature. So we have used all the specifications as they are. Here, we have used UNIFAC as the thermodynamic property package instead of NRTL (used in literature), Because the prediction of the azeotrope point is matching in both case.

For more details about the unit operation specifications and the stream properties, please refer to the flowsheet and literature.

Description of Flowsheet

A stream of flow rate 500 kmol/h containing 20 mol% acetonitrile and 80 mol% water is fed to preconcentration column which produces pure water as a bottom product and a distillate product approaching the azeotropic concentration of MeCN-H_2O mixture (minimum boiling azeotrope of 68% MeCN at 1 atm). Then the distillate product from this column is fed to the 46^{th} stage of the 54 staged extractive distillation column. Ethylene glycol as an entrainer is fed to the column at around 76 ^oC on the 6^{th} stage. The addition of EG alters the relative volatility between MeCN and H_2O, causing MeCN to move towards the top and the mixture of H_2O and EG to be recovered in the bottom of the extractive column. The bottom product of the extractive column is fed to entrainer recovery column to produce almost pure EG as the bottom product and 95% pure H_2O as the top. Heavy entrainer EG is recovered and recycled to the extractive column. A heat exchanger is also employed between extractive distillation column and entrainer recovery column to reduce the temperature to 72 ^oC of recycle stream. A small make-up stream of EG is also fed to the extractive distillation column.

Result

Object	Feed	Pure Water (from Preconcentration Column)	Pure Acetonitrile	Pure Water (from Entrainer Recovery Column)	Pure Ethylene Glycol	Make-up Ethylene Glycol	Unit
Flow Rate	500	348.312	97.7772	53.9111	145.028	0.0086033	**kmol/h**
Acetonitrile	0.2	0.0001	0.99998748	0.04071	0	0	**mol/mol**
Water	0.8	0.9999	0	0.959393	0	0	**mol/mol**
Ethylene Glycol	0	0	0	0	0.9999	1	**mol/mol**

References

[1] W. L. H. L. M. X. a. C. X. Kai Liang, “Energy-Efficient Extractive Distillation Process by Combining,” *Industrial & Engineering Chemistry Research,* 2014.