Process Development for the Production of 10 TPD of Propylene Glycol Monomethyl Ether

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A. Introduction

Propylene Glycol Monomethyl Ether (PGMME) is a methoxy alchohol derivative classified under the p-series glycol ethers. PGMME is largely demanded in the sectors of paints and coatings. It is also known as 1-Methoxy-2-Propanol. It is a colourless and a highly flammable liquid with a molecular formula of $C_4H_{10}O_2$. The major producers of PGMME across the world are Dow Chemicals, Hualun Chemicals and Eastman. Manali Petrochemicals is the dominant producer of PGMME in India. The present work focuses on the production of PGMME by reacting Methanol and PO in the presence of Tri-Ethyl Amine catalyst.

B. Process Flow Sheet Description

The process involves the reaction of Propylene Oxide (PO) and Methanol (MeOH) in the presence of Tri-Ethyl Amine catalyst in a continuous flow reactor. The reaction is exothermic in nature with the formation of a by-product Di-Propylene Glycol Monomethyl Ether (DPGMME). The product stream from the reactor is sent to the first distillation column (Shortcut column, B-6) where large amounts of PO, MeOH and PGMME are recovered at the top along with small traces of DPGMME. DPGMME is removed from the bottom. The distillate stream from the first distillation column (Rigorous distillation column, B-9) wherein the PGMME stream is recovered as bottom. All outlet streams are cooled to ambient temperature

C. Results and Discussion

The process flow sheet was simulated for a plant capacity of 10 TPD of PGMME. The compounds PGMME and DPGMME are presently not available in the Chem-Sep database. Hence, these compounds are created using Joback Group Contribution Method. The Joback

parameters were taken from <u>https://www.chemeo.com/.</u> A conversion reactor was chosen as kinetics of the reaction was not known. The conversion of PO was assumed to be 81% for the first reaction and 9% for the second reaction. In DWSIM, for simultaneous reactions, the conversion should be specified on a sequential basis as described below

Reaction-I (PGMME Formation): 81% (X_1) of Propylene Oxide based on inlet molar flow rate Reaction-II (DPGMME Formation): 9% (X_2) of Propylene Oxide based on inlet molar flow rate

Since the reactions are sequential in DWSIM the second reaction will use the results of the first reaction as a conversion basis. The conversion of PO for Reaction-II was specified using the expression as given below:

Conversion of PO for the formation of DPGMME as per DWSIM = $X_2 * (\frac{100}{100-X_1})$

 X_1 = Percentage conversion of PO for the formation of PGMME based on inlet molar flow rate

 X_2 = Percentage conversion of PO for the formation of DPGMME based on inlet molar flow rate

A shortcut column (B-6) was simulated for the separation of DPGMME with light key compound as MeOH (Composition in Bottoms: 0.0001) and heavy key compound as DPGMME (Composition in Distillate): 0.015919. The reflux ratio was assumed to be 1.5. A rigorous column (B-9) was implemented to separate PGMME and the unreacted reactants. Raoult's law was used as thermodynamic package with Wang-Henke (Bubble-Point) method for the distillation column simulation. The number of stages obtained for the rigorous column was 12 along with a bottoms rate of 432.022 kg/h. All outlet streams were cooled to $25^{\circ}C$

D. Future Work

In the present work the simulation shortcut column (B-6) shows error for certain critical parameters such as reflux ratio, condenser and reboiler duty, since the Lee-Kesler estimation procedure wasn't suitable for DPGMME. In future, this problem can be rectified by using experimental data to simulate the column.