Process Development for Production of 20kTPA of Cumene: Demonstration of closed cycle utility loop

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A. Introduction

Cumene or Isopropylbenzene is an aromatic compound manufactured from propylene and benzene. Essentially most of the cumene produced is further converted to cumene hydroperoxide. Cumene hydroperoxide is an intermediate in the synthesis of other industrially valuable chemicals, such as phenol and acetone. Cumene is a clear colorless liquid with an aromatic odor. Mostly cumene is produced through the Q-max (UoP, Inc.) wherein benzene and propylene are converted to high quality cumene using a zeolite catalyst. In the present work, simulation of a typical cumene production process through direct alkylation of benzene with propylene is performed using a free and open source chemical process simulator.

B. Process Description

Alkylation reaction converts benzene and propylene to cumene and diisopropylbenzene in the presence of the zeolite catalyst. It is an endothermic reaction and occurs at high temperature 250˚C and at atmospheric pressure. The feed stream consisting of 1:1 molar ratio of benzene and propylene is pre-heated to 250˚C and is fed to the reactor. The reaction occurs in the vapor phase. The exit stream from the reactor is cooled to temperature below the boiling point of benzene. The stream is then passed to a flash column operated at vacuum condition of 0.96 atm. The propylene is recovered as vapors stream along with some traces of benzene. Liquid stream from flash column is fed to the primary distillation column. The primary column removes maximum amount of Benzene as distillate. The bottom stream from the primary distillation column is further sent to secondary column to separate Cumene and Diisopropylbenzene. Cumene of 98% purity is obtained as distillate stream. It is then cooled to ambient condition. Steam and water are used as heating and cooling utility streams in the process. Energy recovery is achieved by closed cycle utility loop.

C. Result

The process flow sheet was simulated for the plant capacity of 20kTPA of cumene. Excess amount of benzene increase formation of cumene. The conversion of propylene Oxide was assumed to be 73.5% for cumene reaction and 26.19% for diisopropylbenzene reaction, based on preliminary simulations done with the Gibbs reactor. In DWSIM to simulate multiple reactions, conversion was described on sequential basis as detailed below:

Reaction-I (Cumene Formation): 73.5 % (X_1) of Propylene Oxide based on inlet molar flow rate

Reaction-II (Di-Isopropylbenzene Formation): 26.19 % (X_2) of Propylene Oxide based on inlet molar flow rate

For series reaction in DWSIM, the second reaction will utilize the results of the first reaction as a basis. Hence, the conversion of propylene for Reaction-II was specified using the expression:

Conversion of Propylene for the formation of Di-Isopropylbenzene as per

$$\text{DWSIM} = \frac{100}{100-X_1} * X_2 = 98.9$$

X_1 = Percentage conversion of Propylene for the formation of Cumene based on inlet molar flow rate

X_2 = Percentage conversion of PO for the formation of Di-Isopropylbenzene based on inlet molar flow rate

Shortcut columns (B7 and B9) were simulated to obtain actual of number of stage and minimum reflux ratio. Light key and heavy key components in bottom and top were as 0.001. Minimum reflux ratio and Minimum number of stage for column B7 was found to 0.52 and 9 respectively and for column B9, it is found to be 0.33 and 6 respectively. The result from the shortcut column (B7 and B9) was further used as input to simulate the rigorous distillation column (B-7 and B-9).

D. Conclusion and Suggestion

In the current work process flowsheet was developed and simulated for 20kTPA of cumene with closed loop energy utility cycle. It can be clearly inferred from the simulations that recycle of unreacted benzene reduces amount of fresh feed rate required to meet the target capacity. In the present simulation dealkylation of diisopropylbenzene is not considered. Further work involves incorporation of dealkylation reaction of diisopropylbenzene with benzene to produce cumene and thus further improve the product yield.