Pressure-swing Reactive Distillation Process for Transesterification of Methyl Acetate with Isopropanol

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Introduction

There is a great amount of methyl acetate in production of purified terephthalic acid and Polyvinyl Alcohol. In industry, methyl acetate is generally applied to the production of acetic acid and methanol via hydrolysis. An alternative method to take advantage of methyl acetate is the synthesis of isopropyl acetate via the transesterification reaction of methyl acetate and isopropanol, which is comparatively more attractive.

Reactive distillation (RD) is an innovative process which integrates physical separation and chemical reaction into one unit with less needing of capital investments and operating costs.

The following process leads to formation of an azeotrope of MeOH-MeOAc (66.59 % MeOAc at 1 atm) and in order to separate them Pressure Swing Reactive Distillation (PSRD) has been used. Therefore we have tried to simulate the following PSRD process in a DWSIM Simulator.

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 UNIQUAC (used in literature).

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

Purpose of Study

The reason for using RD here is to reach the desired equilibrium concentration of the product. What happens here is we continuously remove the product in the column and due to Le Chatelier's Principle the reaction would now proceed in forward direction only.

The reason of using pressure swing method is to change the relative volatility and the high pressure (3 atm) increases the percentage of methanol and decreases the percentage of methanol acetate as a result of which the conversion increases and as a result of which percentage MeOAc decreases in distillate as well as bottom product. This leads to low reboiler duty as well as low recycle flow rate from column 2.

Description of Flowsheet

In the PSRD process, there are two columns with different operating pressure. One is a high-pressure column, and another is a low-pressure column. The distillate of the RD column is MeOAc-MeOH mixture, the composition of which is sensitive to the operating pressure. The molar fraction of MeOAc in mixture decreases and the molar fraction of MeOH in mixture increases with the increase of pressure. This means that at higher operating pressure, the reactive conversion can be improved. Thus, the distillate with lower molar fraction of MeOAc in the RD column can be obtained and the lower reboiler duty is needed for obtaining high-purity products in bottoms. Meanwhile, in the RC column, the recycle stream is the MeOAc-MeOH mixture near the azeotropic composition and the recycle flow rate decreases. Therefore, much more energy consumption could be saved with the improvement of the process. It is found that with the operating pressure of 3 atm in RD column, the temperature differentials between the condenser in RD column and the base in RC column is 18℃, which is larger and closest to 15℃ and meets the requirement above. Therefore, the operating pressure for RD and RC columns in PSRD process were chosen on the value of 3atm and 1atm, respectively. In this PSRD process, the base temperature of RC column with 1 atm is 70.61℃

In the flowsheet as Column 1 (RD) operates at 3atm and Column 2 (RC) at 1 atm we have used a valve in order to decrease the pressure.

RD Column- The top temperature of the column is 360 K and the bottom temperature 400K. The reflux ratio maintained here is 5.11

Top Product- MeOH and MeOAc (predominantly), Bottom Product- IPAc

RC Column- The top temperature of the column is 327K and bottom temperature 337K. The reflux ratio maintained is 2.35.

Top Product- MeOH and MeOAc, Bottom Product- MeOH

Result

Object	Pure IPA	Pure MeOAc	Pure IPAc	Pure MeOH	Recycle Stream	Unit
Flow Rate	13.889	13.889	13.7858	13.1816	134.159	**mol/s**
Methanol	0	0	0	0.9837	0.3784	**mol/mol**
Isopropanol	1	0	0.001	0.0162	0	**mol/mol**
Isopropyl Acetate	0	0	0.9874	0	0	**mol/mol**
Methyl Acetate	0	1	0.00115	0	0.621	**mol/mol**

References

[1] Xiaomeng Suo, Qing Ye, Rui Li, Xin Dai, Hao Yu, "The partial heat-integrated pressure-swing reactive distillation process for transesterification of methyl acetate with isopropanol", *Chemical Engineering and Processing*, 2016.