

PRODUCTION OF BUTYL ACETATE AND METHANOL FROM METHYL ACETATE AND BUTANOL

ABSTRACT:

Butyl acetate is an ester used as synthetic fruit flavouring agent. The proposed flowsheet was designed for the production of butyl acetate and a second product methanol from reactants, methyl acetate and butanol. Methanol is generally used as fuel, solvent and antifreeze. This process was simulated using DWSIM open source chemical process simulator. The Lee-Kesler-Plocker property package was chosen as the basis for simulating the entire process. The reaction was executed in a continuously stirred tank reactor of volume 4m³ and the reaction condition of 350 K and 5 atm was maintained.

Keywords –Butyl acetate, reactor, methanol, flavouring agent

INTRODUCTION:

Butyl acetate and methanol are produced by the reaction of methyl acetate with methanol in a reversible, liquid-phase reaction. The reaction is exothermic and the chemical equilibrium constant for this reaction is less than unity and hence there is significant amount of the reactants which is recovered and recycled.

Reaction: MeAc + BuOH -----> MeOH + BuAc

The activation energies are in KJ/mol and the temperature is in K. The overall reaction rate is given as: $R = K_F C_{MeAc} C_{BuOH} - K_R C_{MeOH} C_{BuAc}$

$$K_F = 7 \times 10^6 e^{-71960/RT} ; K_R = 9.467 \times 10^6 e^{-72670/RT}$$

The activation energies are essentially the same, which means that the heat of reaction is small and also that the equilibrium constant decreases only slightly with increasing temperature.

PROCESS DESCRIPTION:

In this process simulation, the reactants, butanol and methyl acetate which were initially maintained at 305K and 15 atm is fed to mixer along with their recycle streams. The reactants were heated to a temperature of 350K and a pressure of about 5 atm. This is fed to a CSTR and the products, butyl acetate and methanol with significant amount of reactants are obtained. This is fed to a distillation column which separates the heavy key components (methanol and methyl acetate) at the top and light key components (butyl acetate and butanol) in the bottom. These streams contains significant amount of impurities. The butanol is separated and recycled. Similarly methyl acetate and methanol is separated and recycled.

RESULTS:

COMPOUNDS	MIXER-1	MIXER-2	REACTOR OUTLET	DISTILLATION TOP	DISTILLATION BOTTOM
MeOH	14.4288	0	14.4894	5.0211	9.4683
BtOH	0	16.687	16.62698	9.41E-20	16.6269
MeAc	21.779	0	21.71846	21.42668	0.2917
BtAc	0	0	0.06064	9.7476E-21	0.06064

TABLE 1: The molar flowrates are given in the above table in mol/s