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STEADY STATE SIMULATION OF ETHYL ACETATE PRODUCTION USING CHEMCAD

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Abstract: *Overall world looking for ethyl acetate as greener fuel. Ethyl acetate is produced by esterification of ethanol and acetic acid. Reactive distillation is column in which combining reaction and separation takes place simultaneously into single column. Sensitive analysis are carried out to investigate the influence of different parameter such as feed stage location, reflux ratio, pressure, reactant etc. The main object of this paper is that obtain high pure ethyl acetate as product. The effect of excess reactant on ethyl acetate also studied. Optimum operating conditions and design parameters of reactive distillation column for high pure ethyl acetate produced is studied.*

Keywords: *Reactive Distillation, CHEMCAD software, Number of stages, Reflux ratio, Purity, Ethyl acetate*

1. Introduction

Reactive distillation operation is gaining lot of attention [1]. Because of the combination of reaction as well as separation in single column work simultaneously. However by reactive distillation can get advantages:- Removal of the product from the reaction mass at the reaction conditions increases equilibrium conversion of reactant, Separate equipment for the separation is not required, Increase the selectivity of product etc.

In this operation, reaction does not affect the separation operation neither does the separation operation affect the reaction. Esterification process is mostly used reactive distillation by using chemcad 6.3.1, developed model and calculations to design of reactive distillation column.

Ethyl acetate is used primarily as a solvent and diluent, being favored because of its low cost, low toxicity, and agreeable odour. For example, it is commonly used to clean circuit boards and in some nail varnish removers (acetone and acetonitrile are also used). Coffee beans and tea leaves are decaffeinated with this solvent. It is also used in paints as an activator or hardener. Ethyl acetate is present in confectionery, perfumes, and fruits. In perfumes, it evaporates quickly, leaving only the scent of the perfume on the skin. Ethyl acetate is used in manufacturing of nail polish remover [2], Explosive [3].Ethyl acetate is produced through esterification of ethyl alcohol and acetic acid. This process is described as an acid catalyzed equilibrium synthesis developed by Emil Fischer [4].

The condition chosen provide the maximum purity upto 99% of ethyl acetate. The reactive distillation setup allows overcoming the reaction equilibrium for increased conversion of ethanol and acetic acid.

The objective of this study is to define reliable reactive distillation model for maximum pure ethyl acetate production. The research provides a comprehensive understanding of the effect of reactant amount excess, feeds stage location, pressure and reflux ratio on the conversion in the reactive distillation, and a demonstration of solution multiplicity in a reactive distillation system for esterification.

2. Objective definition

The main object of this study is to obtain the maximum pure ethyl acetate. So here we have to check all parameters or conditions in optimize manner such as temperature, feed stage location, reflux ratio, composition etc.

3. Thermodynamic requirement

The thermodynamic data required for the phase equilibrium description were obtained in this study on the ground of the K-value methods. The liquid-phase activity coefficients were well represented by the NRTL equation [5].

4. Reaction kinetics

The esterification of acetic acid and ethanol produced ethyl acetate and water by following reaction:

$CH_3CH_2OH+CH_3COOH \rightarrow CH_3COOH_2CH_3+H_2O$

In this reaction, acidic catalyst is added to accelerate the reaction. The reactions parameters are specified on the ground of the experimental data of Nada S. Ahmed Zeki et al. [6]. The values of the activation energy and the pre-exponential factor are obtained at a constant catalyst loading. Thus, the catalyst effect on the reaction kinetic is not taken into account [5].

Reaction kinetics used in the process are:

Activation energy for the first reaction KJ/mole=7150

Value of frequency factor for the first reaction=29000

Activation energy for the second reaction KJ/mole=7150

Value of frequency factor for the second reaction=7380

5. Simulation on chemcad

The SCDS module in ChemCAD 6.3.1 software is used to simulate the reactive distillation process. SCDS is a rigorous multi-stage vapor-liquid equilibrium module which simulates any single column calculation. By this module columns of unlimited stages, five feed streams, and four side products can be simulated[5]. SCDS can simulate rigorous distillation of two-phase or three-phase non-ideal K-value chemical systems [7].

6. Flow sheet

In fig.1, the stream 1 and stream 2 represent feed stream of acetic acid and ethanol respectively. Product out from stream number 3 from the top of the column.

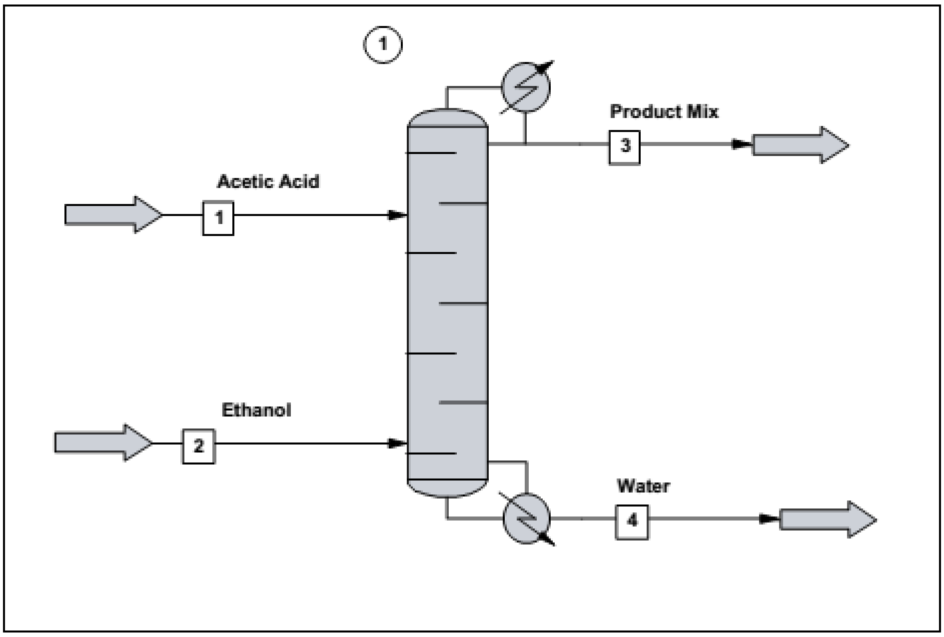

Fig. 1 –Flow sheet

7. Analysis

A. Optimum location of feed stage

Initially one stream keep constant and second stream keep changing upto maximum conversion. After that first stream keep changing and second stream keep constant[8], According to that we get 50 stages column in which acetic acid is fed at the 4th stage while ethanol is fed at the 47th stage for maximum conversion.

Double feeding strategy for reactive distillation column:

Acetic acid feed tray	Ethanol feed tray	Ethyl acetate mole fraction
Tray 4	Tray 44	0.9909
Tray 4	Tray 45	0.9920
Tray 4	Tray 46	0.9921
Tray 4	Tray 47	0.9923

B. Effect of reflux ratio

As we know that if stages of column increases then reflux ratio decreases. So changing the reflux ratio upto maximum concentration of ethyl acetate in product (high pure). Here we get reflux ratio value 16 for maximum ethyl acetate concentration.

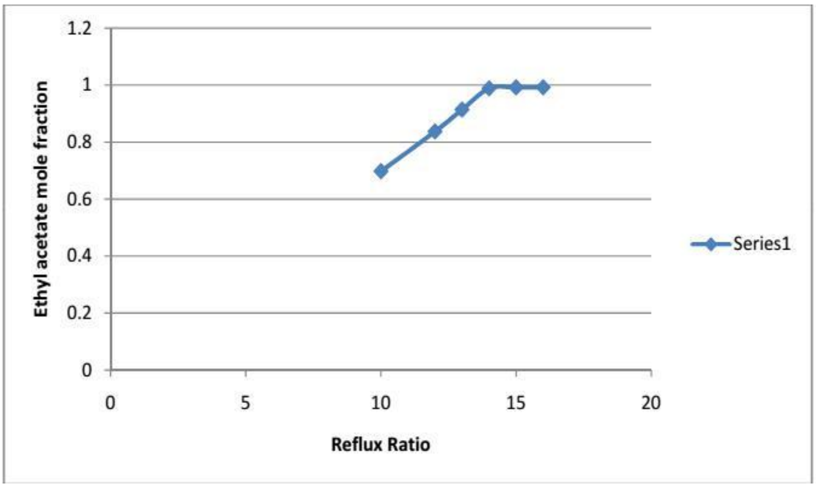

Fig 2 – Reflux ratio vs mole fraction of ethyl acetate

C. Reactant excess

This analysis shows that if changing in reactants concentration then product concentration changes rapidly. Initial flow rates of two reactants, 25(kmol/hr) acetic acid and 25 (kmol/hr) ethanol are set according to stoichiometry of the reaction[5]. So keeping constant flow of ethanol and changing the flow of acetic acid upto getting maximum concentration of ethyl acetate in product stream and vice versa. This analysis shows that 71(kmol/hr) acetic acid flow rate and 15 (kmol/hr) ethanol flow rate for getting maximum purity (99.23%) of ethyl acetate.

D. Effect of pressure

This analysis shows that concentration of ethyl acetate varies with changes in pressure. It shows that if pressure is increase, concentration of ethyl acetate decreases. So we are changing the pressure from 10 bar to 0.5 bar[5]. Below 1 bar means under vacuum cost for operation is higher so we maintained the pressure at 1atm.

E. Temperature profile

It shows that temperature changes in tower from top to bottom. At the top of the column temperature is lower than temperature at the bottom of the column. Because of reboiler at the bottom of the column temperature at lower section of column is lower than upper column. Fig.3 shows that the plot of stage number vs temperature, temperature is higher at bottom.

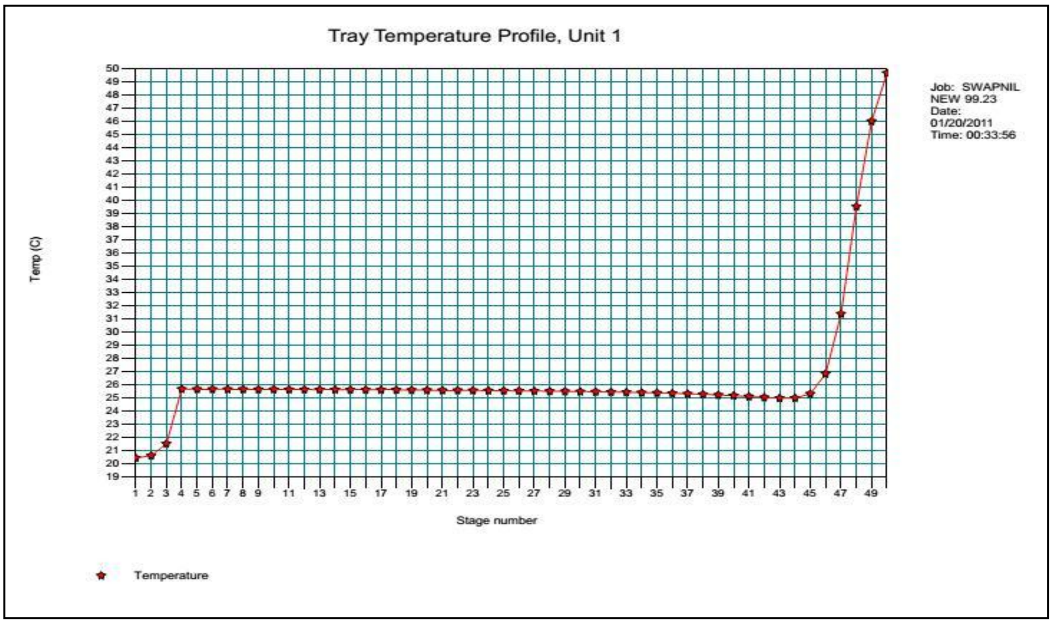

Fig 3 –Temperature profile

8. Result

From the analysis of parameter we can model of reactive distillation column. We get optimum feed stage location, acetic acid is fed to the top of the column at 4th stage and ethanol is fed to the bottom of the column at 47th stage in 50 stages of column. Reactants can used in excess form for high purity of product. So acetic acid is used 71 (kmol/hr) and ethanol is used 15 (kmol/hr). Reflux ratio maintained at value of 16.While pressure is maintained at 1 atm. It is observed from Fig.4 that the maximum composition of ethyl acetate of 0.9923 is obtained at stage 1 corresponding to the total condenser. The trend observed is such that the composition of ethyl acetate reduces in a gradual manner from stage 1 to stage 50.

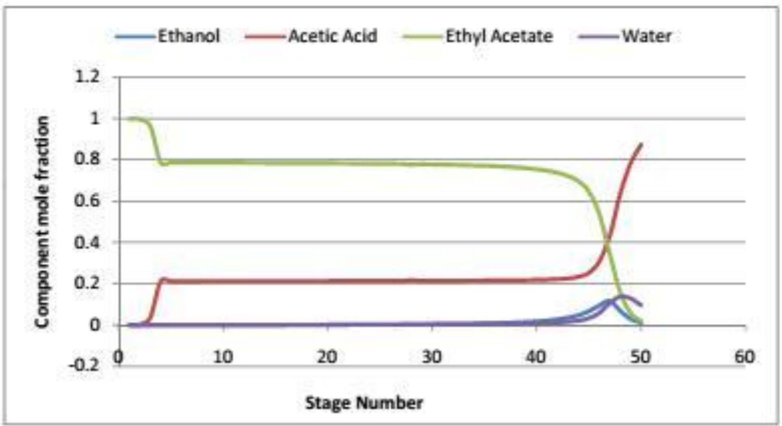

Fig 4-Stage number vs component mole fraction

9. Conclusion

Modelling, simulation and control of an ethyl acetate producing reactive distillation column system was accomplished using commercially available process simulation software, CHEMCAD. Results obtained by simulating the process at steady state show that double feeding strategy gives ethyl acetate with a higher purity. This agrees with the findings of Vora & Daoutidis [9].Who also worked on the same system and reported that top product purity can be improved by feeding reactants in different trays. The optimum location of feed stage was such that acetic acid is fed to stage 4 while ethanol is fed to stage 47. A reflux ratio of 16 resulted in optimum composition of ethyl acetate in the liquid phase and increasing the distillate rate resulted in an increase in the composition of ethyl acetate in the liquid phase. We can recover acetic acid by using extraction column that can be recycled to distillation column.

10. References

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