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Review Modelling of Reactive Distillation Column

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Abstract—*Reactive distillation, i.e. the combination of chemical reaction and distillated product separation in a single unit owing to which itenjoys a number of specific advantages overconventional process or other techniques.Inthis work review on modelling of reactivedistillation for the production of methyl acetatethrough esterification. Methyl acetate and wateris produced by the liquid phase reaction of aceticacid and methanol in the presence of an acid catalyst(e.g. sulfuric acid or a sulfonic acid and ionexchange resin) at 298 K temperature and pressure of 1 atm.In the production of methyl acetate the formation of the low boiling azeotropic mixtures methyl acetate/methanol and methyl acetate/water results in separation ofthese azeotropes is very difficult.This work has been carried out to simulate the conventional and the reactive distillation process methods used for the production of methyl acetate through esterification reaction between acetic acid and methanolusing Aspen Plus. The esterification reaction, occurring in the reactor of the conventional method and inthe reaction section of the reactive distillation method, of the process was modeled as an equilibrium type. Thus the reactive distillation process method was found to be better than the conventional process method.*

1. INTRODUCTION

Methyl acetate, also known as MeOAc, acetic acid methyl ester or methyl ethanoate, is a carboxylate ester with the formula CH_3COOCH_3. It is a flammable liquid with a characteristically pleasant smell reminiscent of some glues and nail polish removers. Methyl acetate is occasionally used as a solvent, being weakly polar and lipophilic, even though its close relative, ethyl acetate, is amore common solvent being less toxic and less soluble in water. Methyl acetate has a solubility of 25% in water at room temperature. At elevated temperature, its solubility in water is much higher.Methyl acetate is produced industrially via the carbonylation of methanol as a byproduct of the production of acetic acid [1].

Reactive distillation operation has been an area of interest from last two decades. The combination of reaction and separation in a single unit is an alternative to conventional distillation which includes reaction and separation in number of units thus increases the investment cost of the plant.The energy requirement of the conventional column is very high and requires large recycling costs. Reactive distillation column works close to the stoichiometric feed conditions thereby eliminating recycling costs and increases the efficiency of the column and conversion.The three important advantages of reactive distillation column are: (i)Distillation column consist of reactive section which leads to the conversion of reactants into products (ii)It improves the separation in the column by changing the component volatilities (iii)increases the selectivity of product [2].

Literature Survey

The process in which reaction zone and separation zone are coupled together is not a newer approach it was patented in 1920's and first real world implementation was done commercially in 1980's. RD has been worked upon by many researchers as Doherty and Buzad, 1992; Podrebarac et. al., 1997.RD is very fortunate in terms of reaction kinetics, economy, yield of product on the other hand its designing is very tedious. Complexity in designing arises due to introduction of in situ separation function within the reaction zone leads to intricate interaction between vapor–liquid equilibria, vapor-liquid mass transfer, intra catalyst diffusion and chemical kinetics [2-3].

Abdulwahab Giwa(2013) had developed an equilibrium model for the production of methyl acetate in "Methyl Acetate Reactive Distillation Process Modelling, Simulation and Optimization using Aspen Plus". The model considered in the simulation was RD column in which reaction takes place in the presence of sulfuric acid and ion exchange resin while the rectification and stripping sections are both filled with Sigma Type and Raschig Type packing [2].

2. PROCEDURES

2.1 Azeotrope Search

Before going into the modeling and simulation of the processes (conventional and reactive distillation), the azeotrope search of the components involved were investigated with the aid of Aspen Plus. In achieving this, the four components (acetic acid, methanol, methyl acetate and water) were considered in their vapor and liquid phases using NRTL Property Model. In addition, a pressure of 1 atm was used.The reason for carrying out the azeotrope search was to establish the significance of applying reactive distillation to this process of ethyl acetate production through Fischer esterification because if no azeotrope was present among the components involved in theprocess, just a simple distillation column coupled with a reactor, instead of reactive distillation,

might be sufficient to produce good yield from the Fischer esterification process. In the production of methyl acetate the formation of the low boiling azeotropic mixtures methyl acetate/methanol (64.5 mol% methyl acetate at 326.8 K) and methyl acetate/water(95 mol% methyl acetate at 330.1 K) results in separation of these azeotropes is very difficult [4].

2.2 Modelling and Simulation

Simulations were carried out using the model

RADFRAC from the commercial steady-state simulator Aspen Plus which is based on a rigorous equilibrium-stage model for solving the MESH equations.

The esterification reaction occurring in the column was modeled as an equilibrium type and it is given as shown in Equation (1) below.

$$CH_3COOH + CH_3OH \overset{K_{eq}}{\longleftrightarrow} CH_3COOCH_3 + H_2O \quad (1)$$

(Abdulwahab Giwa., 2013)

The phase of the reaction was liquid and the basis of the equilibrium constant (Keq) calculated from Gibbs free energy was taken to be molarity [1].

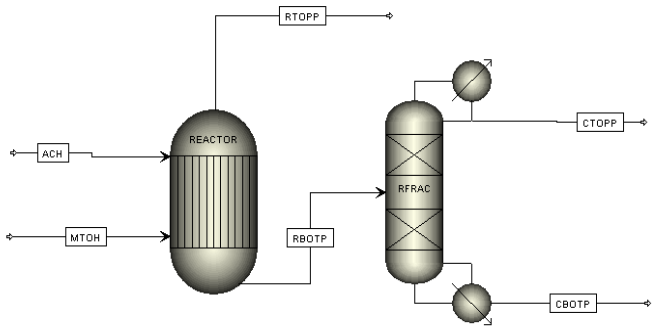

Fig. 1: Aspen Plus model of conventional ethyl acetate production process

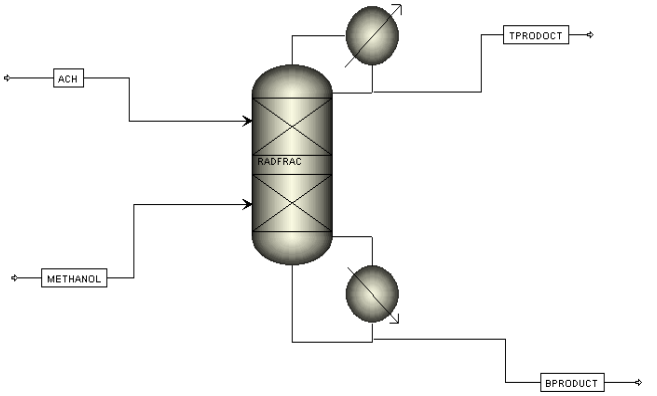

Fig. 2: Aspen Plus model of reactive distillation ethyl acetate production process

The conventional and the reactive distillation process methods used for the production of methyl acetate were modeled and simulated in this work using Aspen Plus. The developed models are as shown in Figures 1 and 2 below respectively for the conventional and the reactive distillation methyl acetate production processes.

The data used for the developments and the simulations of the Aspen Plus models of the conventional and the reactive distillation ethyl acetate production processes are given below in Table 1 and Table 2.

Table 1: Modelling and simulation parametersfor conventional process

Acetic acid	
Flow rate (L/min)	0.05
Temperature (°C)	25
Pressure (atm)	1
Methanol	
Flow rate (L/min)	0.05
Temperature (°C)	25
Pressure (atm)	1
Property method	NRTL
Reaction	
Type	equilibrium
Valid phase	molarity
Temperature (°C)	55
Column	
Type	RADFRAC
No of segments	23
Column feed segments	12
Reflux ratio	3
Reboiler duty (KJ/sec)	0.7
Condenser type	total
Condenser pressure (atm)	1
Packing	raschig

Table 2: Column specification for reactive distillation

Column	
Type	RADFRAC
No of segments	23
Acetic acid feed segment	8
Methanol feed segment	14
Reaction section segments	8-14
Reflux ratio	3
Reboiler duty (KJ/sec)	0.7
Condenser type	total
Condenser pressure (atm)	1
Packing	raschig

At the end of the modeling and simulations, the mole fractions of the components involved in the process especially that of ethyl acetate, which was the desired product of the process, obtained from the two process methods were compared [5].

3. RESULTS AND DISCUSSION

The temperature profile of the simulation carriedout for the production of methyl acetate (desired product) and water (by-product) using the esterification reaction between acetic acid and methanol, with the aid of Aspen PLUS, is given in Figure-3.
Shown in Fig. 3 are the temperature profiles obtained from the simulations of the conventional and the reactive distillation Aspen Plus models of the Fischer esterification used for methyl acetate production. As can be observed from the figure, the profiles of the two process methods were found to be entirely very different from each other especially in the rectifying and the reaction sections of the columns, even though their behaviors were similar in the stripping sections of the columns.Looking at the profile of the reactive distillation process given in Fig. 3, high temperatures were observed to occur at the reaction section. This high temperature given by the reactive distillation process in the reaction section was discovered to be as a result of the exothermic reaction occurring in that section of the column. Such high temperatures were, however, not observed to occur in the case of the column profile of the conventional process method because, in this case, the column was only used for separation, but not for simultaneous reaction and separation.

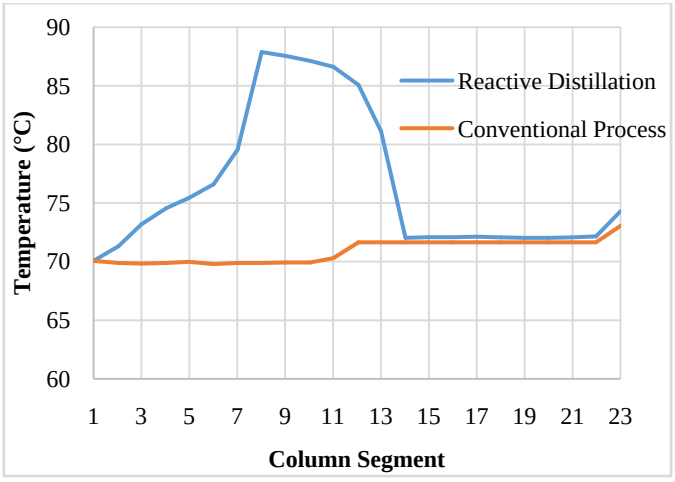

Fig. 3: Conventional and reactive distillation methyl acetate production process temperature profiles

The mole fraction profiles of acetic acid obtained from the Aspen Plus simulations of the conventional and the reactive distillation process methods are as shown in Fig. 4. The trends of the profiles were found to be similar to those of the temperature profiles of the process methods. According to the figure, the mole fractions of acetic acid obtained from the condenser segments of the columns were found to be approximately the same and very close to zero. This was an indication that good separation phenomena were achieved in the columns because, acetic acid, being the heaviest components of the process, was expected to be present in the top segments of the columns in very negligible amounts.As can be seen from Fig. 4, no such high acetic acid mole fraction was observed in the case of the conventional process method because, in this case, there was not any continuous feed of acetic acid being passed into the column.

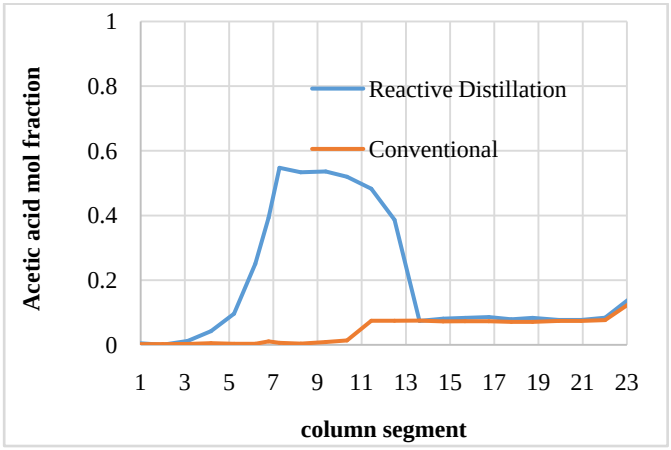

Fig. 4: Conventional and reactive distillation liquid acetic acid composition profiles

Given in Fig. 5 are the liquid mole fractions of methanol obtained from the simulations of the conventional and the reactive distillation processes. From the figure, the mole fraction profile of methanol obtained from the conventional process method was found to be almost constant along all the segments of the column while that of the reactive distillation process method was only almost constant from the top segment of the column up to about segment 13, thereafter, there was an increase in the mole fraction a bit, which later decreased again a bit.As can be observed from the profiles of the reactive distillation and the conventional process, used for the production of methyl acetate through Fischer esterification, given in Fig. 5, in the top segments of the columns, the mole fraction of ethanol given by the reactive distillation process method was found to be less than that of the conventional process method.

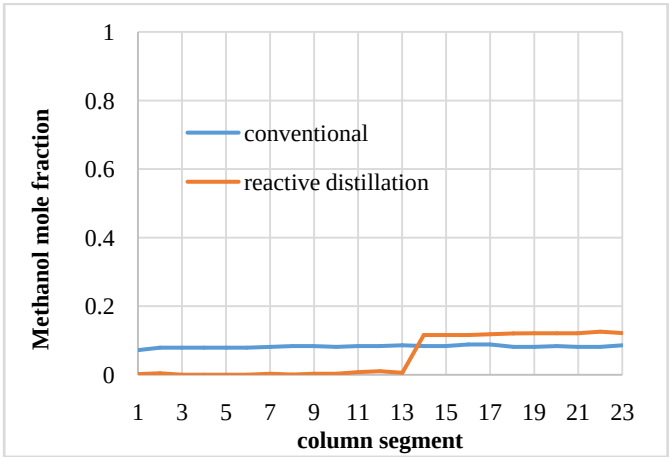

Fig. 5: Conventional and reactive distillation liquid methanol composition profiles

Now, in Fig. 6, the liquid mole fraction profiles of the desired product (methyl acetate) obtained from the simulations of the conventional and the reactive distillationprocess methods are given. Considering the results given in the Fig. (Fig. 6), the methyl acetate that was obtained from the reactive distillation process method was found to have higher mole fraction in the top segment (condenser) of the column than that given by the conventional process method. In the reboiler (bottom segment) of the column, methyl acetate with the lower mole fraction was discovered to be the one obtained from the reactive distillation process method. That is to say, employing reactive distillation process method, higher mole fraction of the desired product (methyl acetate) than that obtained from the conventional process method could be obtained. Another interesting thing that was noticed in the case of the reactive distillation process method, as shown in its profile given in Fig. 6, was that the maximum mole fraction of methyl acetate present in the column was 0.9283.In the case of the conventional process method because the mole fraction of methyl acetate obtained from the condenser of the column of the conventional method had approximately the same mole fraction with that of the one present in each segment of itsrectifying column.

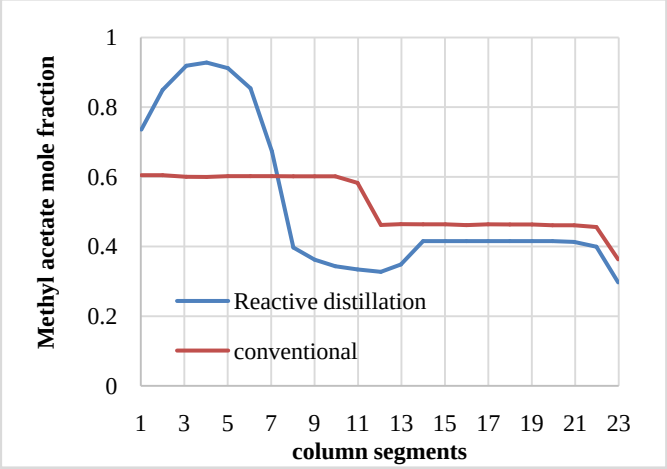

Fig. 6: Conventional and reactive distillation methyl acetate production process temperature profiles

So far, reactive distillation process method has been seen to give higher mole fraction of the desired product (methyl acetate) of this esterification process than the conventional process method. As such, reactive distillation process method has been proved to be better than conventional process method in the production of methyl acetate from the equilibrium esterification reaction between acetic acid and methanol.

4. CONCLUSION

The good convergence obtained from the simulation of the Aspen PLUS model developed for the reactive distillation esterification process used for the production of methyl acetate has shown the versatility of Aspen PLUS in successfully representing the behavior ofthe complex reactive distillation process. Thus the reactive distillation process method was found to be better than the conventional process method.

5. ACKNOWLEDGEMENT

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REFERENCES

[1] Abdulwahab GIWA, “METHYL ACETATE REACTIVE DISTILLATION PROCESS MODELING,SIMULATION AND OPTIMIZATION USING ASPEN PLUS”, ARPN Journal of Engineering and Applied Sciences, 8, 5, May 2013.

[2] R. Taylor, R. Krishna, “Review Modelling reactive distillation”, Chemical Engineering Science, 55, (2000), 5183-5229.

[3] Shivali Arora, Prashant Srivastava, “Review Modeling of Reactive Distillation Column for the Production of Ethyl Acetate through Esterification”, International Journal of Science and Research, 2012.

[4] Sohail Rasool Lone,Syed Akhlaq Ahmad, “Modeling and Simulation of Ethyl Acetate Reactive Distillation Column Using Aspen Plus”, International Journal Of Scientific & Engineering Research, 8,August-2012.

[5] Tim Popken, Sven Steinigeweg, and Jurgen Gmehling, “Synthesis and Hydrolysis of Methyl Acetate by Reactive Distillation Using Structured Catalytic Packings: Experiments and Simulation”, Ind. Eng. Chem. Resarch, 40, 2001,1566-1574.