Indian Journal of Chemical Technology
Vol. 33, January 2026, pp. 110-119
DOI: 10.56042/ijct.v33i1.17395

A comparative study of equilibrium and non-equilibrium models for ethyl acetate production in reactive distillation

Mallaiah Mekala*
Department of Chemical Engineering, Chaitanya Bharathi Institute of Technology, Hyderabad, 500075, India
*E-mail: mmyadav2001@gmail.com

Received 23 February 2025; accepted 13 October 2025

The mathematical modeling and simulation have been performed to an esterification of Acetic Acid (AA) with Ethyl Alcohol (EOH) for production of Ethyl Acetate (EA) and water in a Reactive Distillation Column (RDC). The equilibrium and non-equilibrium (rate based) models have been applied to perform simulations for an esterification system. The ethyl alcohol and acetic acid reacts with sulphuric acidin reactive zone for the production of ethyl acetate and water. The in-situ separations of components in reaction section improves conversion and purity. The feeds entered into the column are at a temperature of 25ºC and a pressure of 1 bar. The feed flow rates are adjusted from 0.02 L/min to 0.09 L/min. The acetic acid is fed on 8th stage and ethanol is fed on 14th stage. The composition and temperature profiles have compared for the equilibrium and rate based models from condenser stage to reboiler stage. Sensitivity analysis was performed under various operating conditions for the equilibrium and rate based models. From the simulations it is found that mole fraction of ethyl acetate is 71.41% from rate based model which is higher than equilibrium model.

Keywords: Catalyst, Equilibrium model, Reactive Distillation, Rate based model, Sensitivity Analysis

Introduction

The integration of reaction and distillation process within the same unit is known as Reactive Distillation (RD). Reactive distillation is a process which combines both reactor and distillation in a single column. As a result, both the process occurs at the same time in one unit. It is challenging task to maintain high reactant concentrations in the reactive zone as well as separation of the products from the column[1-3].

RD also known as catalytic distillation when the solid catalyst is placed in reactive section. This unit is applicable for equilibrium limited reactions where products are continuously removed from the reaction section. Hence the overall conversion of this kind of reactions increases drastically by shifting the forward reaction towards product side.

In RD, the use of excess reactants are reduced like in conventional process to increase the reactant conversion. This method is particularly beneficial for equilibrium limited reaction systems, such as etherification, esterification, hydrolysis and polymerization. In reactive distillation, products are continuously removed from the reactive zone which can enhances conversion of limiting reactant. It has a significant influence by lowering capital costs[4-6]. The application of RD depends on volatilities of reactants and products and matching of reaction and separation temperature in the column.

The production of ethyl acetate (EA) in the RD has advantages compared to conventional method. In conventional method, it has less conversion and requires large capital and energy costs. In reactive distillation, the ethyl acetate has high conversion of limiting reactant, less capital cost and energy requirements are advantage compared to conventional method[7-9].

The reaction between ethyl alcohol (EOH) and acetic acid (AA) to produce EA and water in presence of catalyst is given below.

$$CH_3COOH + C_2H_5OH \leftrightarrow C_2H_5COOCH_3 + H_2O \quad \ldots (1)$$

The modelling and simulations of esterification of AA with EOH in reactive distillation was carried out by Sohail *et al.*[10] using Aspen Plus. The authors applied RADFRAC model for the simulation studies under various parameters. The simulation results with RADFRAC model assumption and literature data are matched well for the EA process.

Ruining *et al.*[11] have investigated the kinetics and simulations for the esterification of AA with EOH in presence of ionic liquid as green catalysts. The reaction kinetics data was used for the development of ideal homogeneous and non-ideal homogeneous kinetic models. The effects of different conditions like temperature, catalyst amount and reactant initial ratio were analysed. The simulations have performed for the esterification system under different conditions, catalyst amount, reflux ratio, feed location and number of theoretical stages on conversion and purity of EOH and EA respectively. They found that EOH conversion of 91.51% and EA purity of 98.94% in an industrial scale reactive distillation process.

Abdulwahab *et al.*[12] have performed the simulations and economic analysis for the production of EA in Aspen Plus environment in conventional and reactive distillation modes. They presumed an equilibrium stage wise model to perform sensitivity analysis. The highest mole fraction of EA in the distillate was 0.9283. From the economic analysis, they found that the cost of reactive distillation was less than conventional process by 17%.

Kiss *et al.*[13] have investigated an overview of reactive distillation process for various systems. The author discussed the production of acrylic and methacrylic monomers, fatty esters, di-alkyl ethers, unsaturated polyesters resins and others. The advantages of RD was highlighted in their study.

Chavdar and Evgeni[14] have investigated esterification of acetic acid with ethanol to produce ethyl acetate in a reactive distillation. The technological approach was designed to save energy by allowing heat recovery from the reboiler stream. The sensitivity analyses have performed for maximum amount of ethyl acetate and minima reboiler heat duty with optimal purity of the water flow. From their investigations, maximum ethyl acetate mole fraction in the distillate obtained when acid feed introduced above 10th stage and ethanol is below 13th stage. The reflux ratio and mole ratio of ethanol to acid was 4 and 2.04, respectively. Mayra *et al.*[15] have proposed a heterogeneously catalysed reactive distillation column at pilot scale level to produce ethyl acetate from the esterification of acetic acid and ethanol.

Branislav[16] have proposed a multi aspect comparison of ethyl acetate production in process integration and intensification methods. They have considered four types of process integration methods to steady the conversion as well as purity of ethyl acetate. The energy savings and cost analysis were investigated. The different process namely, conventional process set-up; reactive distillation column with a separation unit, reactive distillation column with a stripper, and Reactive Distillation column with an Auxiliary Reaction (RDAR). A multi-aspect comparison of the set-ups covering energy requirements, economy, and safety analysis was done. The lowest energy consumption was achieved in a fully integrated and intensified process, due to the synergy of two chemical reactions and enhanced product separation.

Miguel *et al.*[17] have proposed a dividing wall reactive distillation for EA production and compared the conversion and purity of AA and EA conventional and reactive distillation methods. The authors found that with dividing wall reactive distillation 46% energy and 26% cost savings compared with the traditional process.

The present study deals with the comparison of equilibrium and non-equilibrium models for the EA production. Very few studies are available for the comparison of these models for EA production. The various thermodynamic models used for this process in RD but no literature available for EA production in RD with UNIFAC thermodynamic model. In the present study, the equilibrium and non-equilibrium models are developed and simulations have performed for EA production in the RD column. The sensitivity analysis has performed under various parameters of flow rates, mole ratio and reflux ratio for equilibrium and non-equilibrium (rate based) models for the purity of ethyl acetate in distillate.

Mathematical Modelling

The present study, the equilibrium and rate based modelling approaches are used for simulation of EA production in the reactive distillation.

Equilibrium model

Mass and energy balance equations are applied to equilibrium model for reactive distillation column. It is also considered that compositions are equilibrium on each stage. HETP is mentioned for each type of packing and same is considered. Aspen Plus software 11.2 version is used for simulations.

The equilibrium model equations for solving the mass and energy balances are as follows[18].

Model equations for condenser

Molar balance for components

$$V_2 y_{i,2} - L_1 x_{i,1} - D x_{i,1} = 0 \qquad \dots (2)$$

Total enthalpy balance

$$V_2 H_2^{Vap} - L_1 H_1^{Liq} - D H_1^{Liq} - Q_{Condenser} = 0 \quad \ldots (3)$$

Total composition is unity

$$\sum_{i=1}^{NC} \left(x_{i,1} \right) = 1 \quad \ldots (4)$$

Model equations for the reboiler
Molar balance for components

$$L_{N-1} x_{i,N-1} - L_N x_{i,N} - V_N y_{i,N} = 0 \quad \ldots (5)$$

Total energy/enthalpy balance

$$L_{N-1} H_{N-1}^{Liq} - L_N H_N^{Liq} - V_N H_N^{Vap} + Q_{\mathrm{Re}boiler} = 0 \quad \ldots (6)$$

Total composition is unity

$$\sum_{i=1}^{NC} \left(x_{i,N} \right) = 1 \quad \ldots (7)$$

$$\sum_{i=1}^{NC} \left(y_{i,N} \right) = 1 \quad \ldots (8)$$

VLE relation

$$y_{i,N} = \left(K_{i,N} x_{i,N} \right) \quad \ldots (9)$$

jth stage model equations
Component balance on molar basis

$$L_{j-1} x_{i,j-1} - L_j x_{i,j} + V_{j+1} y_{i,j+1} - V_j y_{i,j} + \varepsilon_j R_{i,j} = 0 \quad \ldots (10)$$

To Feed

$$L_{j-1} x_{i,j-1} - L_j x_{i,j} + F_j Z_{i,j}^F + V_{j+1} y_{i,j+1} - V_j y_{i,j} + \varepsilon_j R_{i,j} = 0 \quad \ldots (11)$$

Total enthalpy balance

$$\left(L_{j-1} H_{j-1}^{Liq} - L_j H_j^{Liq} + V_{j+1} H_{j+1}^{Vap} - V_j H_j^{Vap} \right) = 0 \quad \ldots (12)$$

For feed stage

$$L_{j-1} H_{j-1}^{Liq} + F_j h_j^F - L_j H_j^{Liq} + V_{j+1} H_{j+1}^{Vap} - V_j H_j^{Vap} = 0 \quad \ldots (13)$$

Total composition is unity

$$\sum_{i=1}^{NC} \left(x_{i,j} \right) = 1 \quad \ldots (14)$$

$$\sum_{i=1}^{NC} \left(y_{i,j} \right) = 1 \quad \ldots (15)$$

VLE relation

$$y_{i,j} = \left(K_{i,j} x_{i,j} \right) \quad \ldots (16)$$

Non equilibrium stage model

Non-equilibrium model also known as Rate Based (RB) model. The non-equilibrium model considered based on interface mass as well as heat transfer calculations with transport expressions instead of stage wise model. Further assumption is VLE exist at interface only. The reaction occurs in liquid phase and the rate expression was used from Zeki *et al.*[19]. This rate equation used in both the models for simulation studies. In the non-equilibrium model, mass and energy balance equations are applied to liquid and vapour phases separately and these are given below[20].

Total condenser
Molar component balance

$$M_{i,1} = V_2 y_{i,2} - L_1 x_{i,1} - D x_{i,1} = 0 \quad \ldots (17)$$

Total energy balance

$$V_2 H_2^{Vap} - L_1 H_1^{Liq} - D H_1^{Liq} - Q_{Condenser} = 0 \quad \ldots (18)$$

Total composition is unity

$$\sum_{i=1}^{NC} \left(x_{i,1} \right) = 1 \quad \ldots (19)$$

Reboiler
Molar component balance

$$M_{i,N} = L_{N-1} x_{i,N-1} - L_N x_{i,N} - V_N y_{i,N} = 0 \quad \ldots (20)$$

Total energy balance

$$L_{N-1} H_{N-1}^{Liq} - L_N H_N^{Liq} - V_N h_N^{Vap} + Q_{\mathrm{Re}boiler} = 0 \quad \ldots (21)$$

Total composition is unity

$$\sum_{i=1}^{NC}\left(x_{i,N}\right)=1 \qquad \ldots (22)$$

$$\sum_{i=1}^{NC}\left(y_{i,N}\right)=1 \qquad \ldots (23)$$

VLE relation

$$y_{i,N}=\left(K_{i,N}x_{i,N}\right) \qquad \ldots (24)$$

To jth stage

For liquid phase molar balance

$$M_{i,j}^{Liq}=F_{i,j}^{Liq}x_F^L-N_{i,j}^{Liq}+rxn_{i,j}U_j+L_{i,j-1}x_{i,j-1}-L_{i,j}x_{i,j}=0 \qquad \ldots (25)$$

Where U_j is holdup of reaction of jth stage, N_i^L is mass flux of the ith component at interface.

$$N_{i,j}^{Liq}=k_{i,j}^{Liq}a_j\left(x_{i,j}^{IP}-x_{k,j}\right)+N_j^{Liq}x_{i,j}^{IP} \qquad \ldots (26)$$

For the vapour phase jth stage molar balance is

$$M_{i,j}^{Vap}=F_{i,j}^{Vap}x_F^{Vap}-V_{i,j}y_{i,j}+V_{i,j+1}y_{i,j+1}-N_{i,j}^{Vap}=0 \qquad \ldots (27)$$

From V pahse to I phase, mass flux is

$$N_{i,j}^{Vap}=k_{i,j}^{Vap}a_j\left(y_{i,j}-y_{i,j}^{IP}\right)+N_j^{Vap}y_{i,j}^{IP} \qquad \ldots (28)$$

Energy balance for liquid phase is

$$E_j^{Liq}=L_{j-1}H_{j-1}^{Liq}+\left(\sum_{i=1}^{c}F_{i,j}^{Liq}\right)H_j^{LF}-H_j^{Liq}+h_j^La_j\left(T_j^I-T_j^{Liq}\right)+N_j^{Liq}H_j^{Liq}=0 \qquad \ldots (29)$$

Energy balance equation for vapour is

$$E_j^{Vap}=V_{j+1}H_{j+1}^{Vap}+\left(\sum_{i=1}^{c}F_{ij}^{Vap}\right)H_j^{VF}-h_j^{Vap}a_j\left(T_j^{Vap}-T_j^I\right)-N_j^{Vap}H_j^{Vap}=0 \qquad \ldots (30)$$

At interface,

$$M_{i,j}^I=N_{i,j}^{Liq}-N_{i,j}^{Vap}=0 \qquad \ldots (31)$$

$$E_j^I=h_j^{Vap}\left(T_j^{Vap}-T_j^I\right)-h_j^{Liq}\left(T_j^I-T_j^{Liq}\right)+N_j^{Vap}H_j^{Vap}-N_j^{Liq}H_j^{Liq}=0 \qquad \ldots (32)$$

At interface

$$K_{ij}x_{ij}^I-y_{ij}^I=0 \qquad \ldots (33)$$

Mass and heat transfer coefficients for the multi-components are calculated according to Taylor and Krishna approach[21]. The reaction rates are calculated by Zeki *et al.*[19]. The UNIFAC model is used for non-ideality of the solution.

The homogeneous second order non ideal kinetic equation is assumed. The kinetic parameters taken from Zeki *et al.*[19]. The activation energy and the pre-exponential factor are 34576 J/mol and 52313 J/mol, respectively. These parameter indirectly linked to sulphuric acid catalyst activity.

The multicomponent mixture contains EOH, AA, water and EA forms azeotropes at certain composition and temperature. The azeotropic compositions in the EA system is given in Table 1

Results and Discussion

The simulations have been carried out for AA and EOH esterification with sulphuric acid in RD using equilibrium and non-equilibrium models. Fig. 1 represents the main flow sheet of Aspen Plus simulation of reactive distillation column. Condenser and reboiler are considered as top and bottom stages. Both the reactants are entered into the column above and below the reactive zone. The products EA and

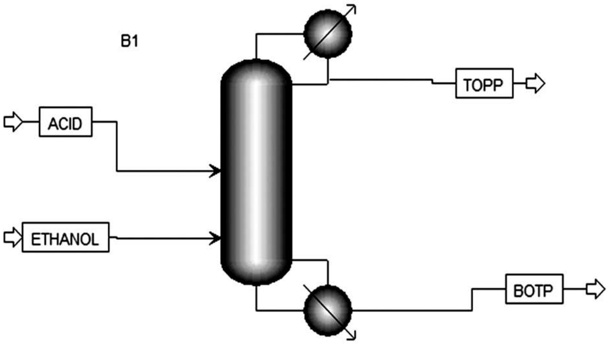

Fig. 1 — Main flow sheet of reactive distillation

Table 1 – Azeotropic compositions in the ethyl acetate system[22]

Reactant and Products combination	T(K)	Azeotrope type	Composition		
			Ethyl Acetate	Ethyl Alcohol	Water
Ethyl Acetate and Ethyl Alcohol	344.77	Homo	0.552	0.448	0
Water and Ethyl alcohol	351.14	Homo	0	0.892	0.108
Ethyl Acetate and Water	344.24	Hetero	0.676	0	0.324
Ethyl alcohol, Ethyl Acetate and Water	343.45	Homo	0.558	0.151	0.291

water produced in reactive zone. The EA is separated from the reactive zone to rectifying zone and finally collected as a product in the distillate. Water is separated from the reactive zone to stripping zone and collected in the reboiler as bottoms.

The simulations have been performed in Aspen Plus with equilibrium and non-equilibrium stage modelling approach[3,7,23] for the esterification process. According to the specifications of equivalent reactive and non-reactive packing, the reactive distillation contains 23 stages including condenser and reboiler. The column stages are counted from top to bottom. Condenser and reboiler are 1st and 23rd stage. The enriching section: 2nd to 7th; stripping section: 15th to 22nd. The AA and EOH are located on 8th and 14th stages, respectively. Table 2 shows the process parameters were used for simulations. The comparison of simulation results for both the models is shown in the following sections.

Temperature versus number of stages

Fig. 2 shows the simulation results of temperature profiles with respect to stage number for equilibrium and rate based models. From the Fig. 2, it can observe that there is a sudden increase of temperature from the stage 1 to stage 5 in equilibrium model compared to rate-based model. It goes on increasing till 8th stage for both cases. The increase in temperature is due to the exothermic reaction which occurs in the reactive section and releases the heat in the reactive zone in addition to reboiler heat duty. Then the temperature gradually decreases till 14th stage and becomes constant for the remaining stages.

Table 2 — Process parameetrs for simulation study

Parameter	Equilibrium	Rate based
Feed conditions: Acetic acid		
Volumetric flow rate	0.06 L/min	0.04 L/min
T	25°C	25°C
P	1bar	1 bar
Feed Conditions : Ethyl alcohol		
Flow rate	0.06 L/min	0.04 L/min
Temperature	25°C	25°C
Pressure	1 bar	1 bar
Property method	UNIFAC	UNIFAC
RD Column		
Stages	23	23
Reflux ratio	1	1
Acetic feed segment	8	8
Ethanol feed segment	14	14
Reboiler duty	0.7 kJ/s	0.7 kJ/s

Composition versus number of stages

The composition data obtained from simulations for equilibrium and non-equilibrium models are shown in Fig. 3. From stages 1 to 5, EA composition is more and water composition is less. The ethyl acetate composition is decreasing and water composition is increasing from stage 7 to sage 14 due to addition of reactants in the reactive portion which enhances rate of reaction. In reactive zone reactants concentration is more hence products composition is less. The water composition increases from stage 14 to stage 23 since water has high boiling point and less volatility. Water composition is increases in the column. From the figure can see that ethyl acetate composition is more in the non-equilibrium model compared to equilibrium model.

Mole fraction of ethyl acetate versus number of stages

The simulation results of EA mole fraction versus stage number is shown in Fig. 4. From the Fig.4, it is observed that there is more deviation in ethyl acetate composition between equilibrium and non-equilibrium models. EA composition is gradually decreases from

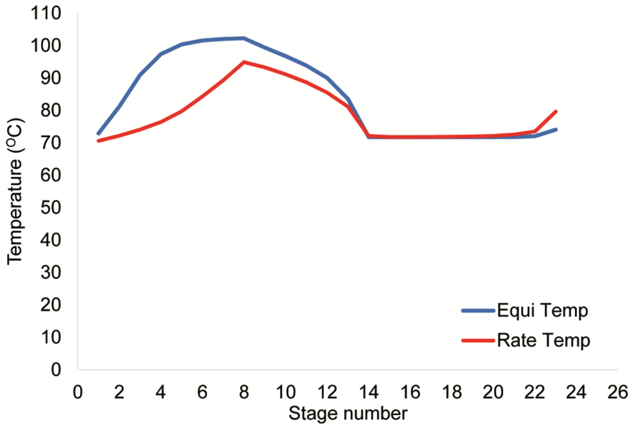

Fig. 2 — Temperature profile as function of number of stages

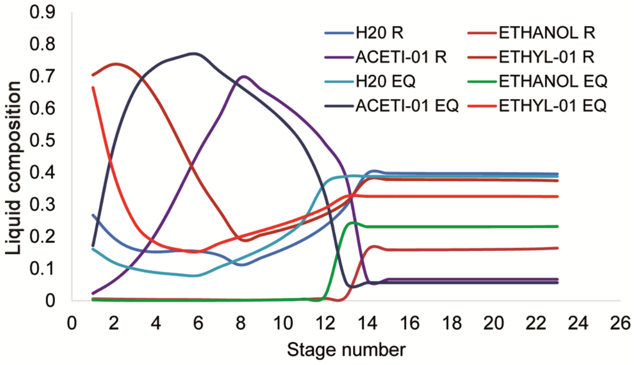

Fig. 3 — Liquid composition profiles as function of number of stages

condenser stage to reactive zone for RB model. EA composition is suddenly decreases from condenser stage to reactive zone in the case of equilibrium model. After reaching 6th stage, ethyl acetate composition is increases till the 14th stage. It is due to reaction between acetic acid and ethanol in reactive section increases the product formation, hence EA composition is increased in both the cases. In the stripping section/zone ethyl acetate composition maintained constant and rate based model has more composition of ethyl acetate compared to equilibrium model. It can observed that the composition of ethyl acetate is more in rate based model which is 71.41% whereas in equilibrium based model it is around is 66.45%.

Mole fraction of water versus number of stages

The simulation results of water mole fraction against the stage number are shown in Fig. 5. It is observed that there is a deviation in water composition between these models. Water composition is gradually decreases from condenser stage to reactive zone in the case of RB model. Water composition is slowly decreases from condenser stage to reactive zone in the case of equilibrium model. After reaching 6th stage, water composition is increases till 14th stage. It is due to reaction between AA and EOH in reactive portion increases product formation, hence water composition is increased in both the cases. In the stripping section/zone water composition maintained constant and rate based model has more composition of water compared to equilibrium model. It can observe that the composition of water is more in rate based model which is 39.71% whereas in equilibrium based model it is around is 38.72%.

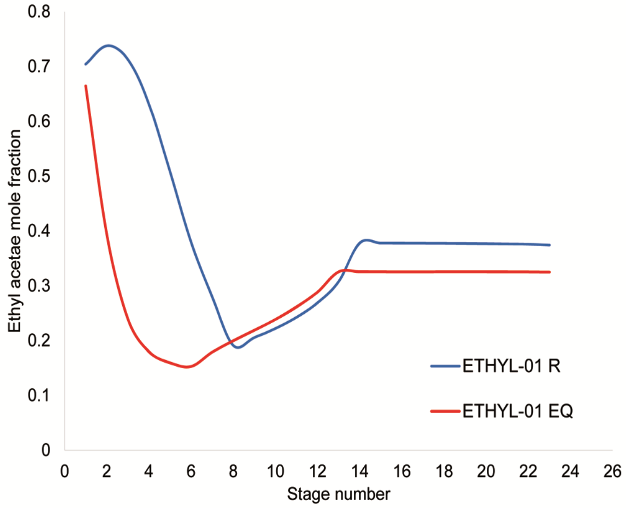

Fig. 4 — Mole fraction of ethyl acetate versus number of stages

K-value versus number of stages

The K-values obtained for ethyl acetate against the number of stages is shown in Fig. 6. It is observed that K-value increases slowly in non-equilibrium model and increases rapidly in equilibrium model. The K-values becomes constant from 14thto 18th stage and K-values raised rapidly in RB model whereas there is not much increase in the equilibrium model. The UNIFAC thermodynamic model is able to predict the accurate results for both the models. From Fig. 6, it is observed that rate-based model K-values are more than equilibrium model. Thus, it can be concluded that in rate based model has maximum conversion and purity.

Liquid flow rates versus number of stages

Fig. 7 shows the comparison of liquid flow rates versus stage numbers for rate based and equilibrium model simulations. From the Fig.7, it can see that

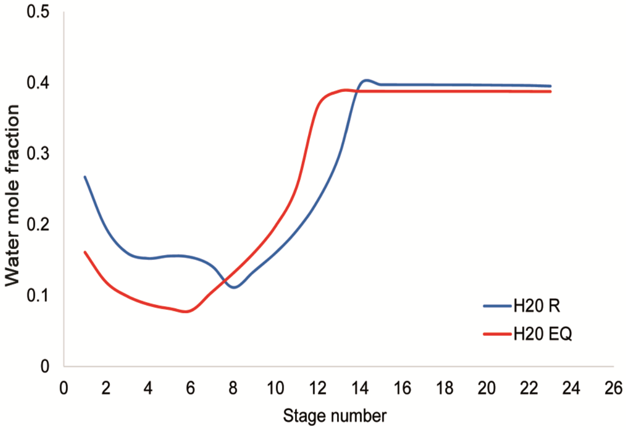

Fig.5 — Mole fraction of water versus number of stages

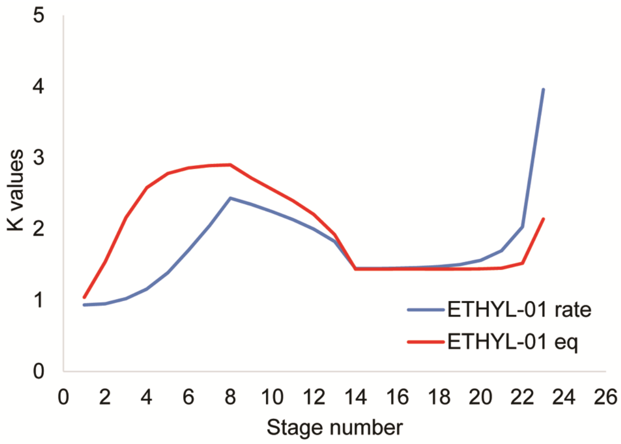

Fig.6 — K- value versus number of stages

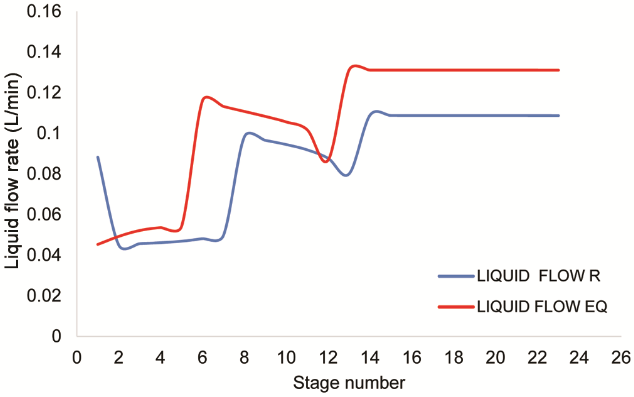

Fig 7 — Liquid flow rates versus number of stages

liquid flow rates are decreasing from condenser stage to 1st stage and increases 3rd stage to 6th stage for rate based model. In equilibrium model, flow rates are increases from 1st stage and 6th stage. The flow rates are maintained constant more or less in the reactive zone. Later liquid flow rates are decreases and again increases and remains constant in the stripping section because of more vaporization rate.

Sensitivity Analysis

Sensitivity analysis has been performed for ethyl acetate production in RD for both the models.

Volumetric flow rate

The composition of EA will be influenced by the altering volumetric flow rates of the reactants into column. The varying feed flow rates will influence the conversion and purity of EA in distillate.

Rate based model

The sensitivity analysis of effect of volumetric flow rate on ethyl acetate production is shown in Fig. 8a. It can observe that as the volumetric flow rate is increases, the mole fraction of ethyl acetate also increases till 0.04 L/min flow rate; after that it decreases. This is because when volumetric flow rate is increases there is a sufficient contact of reactants with catalyst. When the flow rate is high then contact time of reactants and catalyst inside reactive zone is less. Only less amount of ethyl acetate is formed at high reactants flow rates into the column.

Equilibrium model

Fig. 8b shows volumetric flow rate effect on ethyl acetate production for equilibrium model. As volumetric flow rate increases, ethyl acetate mole fraction decreases. As volumetric flow rate is increasing contact between reactants and catalyst inside the packing is more hence high purity of desired product formation. When rate flow is higher than required rate; then the contact time of reactants and catalyst is less and less product formation. Hence, maintaining 0.04 L/min volumetric flow rate would give higher ethyl acetate composition in the distillate.

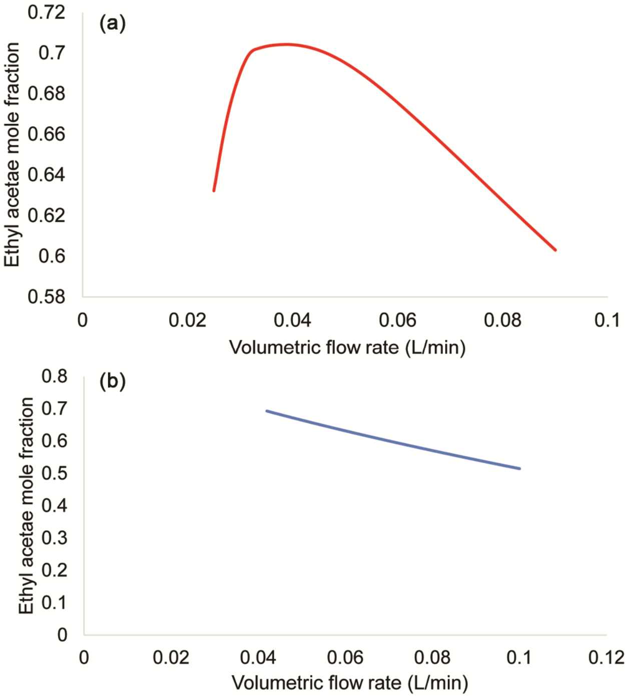

Fig. 8 — Effect of volumetric flow rate for (a) rate-based and (b) equilibrium based on ethyl acetate production

Mole – RR

The reflux ratio is one of key parameter in RDC to improve the purity of ethyl acetate.

Rate based model

Effect of mole-RR on ethyl acetate production by rate-based model prediction is shown in Fig. 9a. From the sensitivity analysis it can observe that when reflux ratio increased there is increase in ethyl acetate production and reaches maximum level and then decreases when there is further increase of reflux ratio. At a reflux ratio of 1.5, EA mole fraction in distillate is 73 %. The ethyl acetate mole fraction decreases further increase in reflux ratio. This is due to further increase in reflux ratio causes insufficient contact of reactants with catalyst as well of less mass transfer between the vapour and liquid phases occurs. The optimum reflux ratio is 1.5 which gives more production of ethyl acetate.

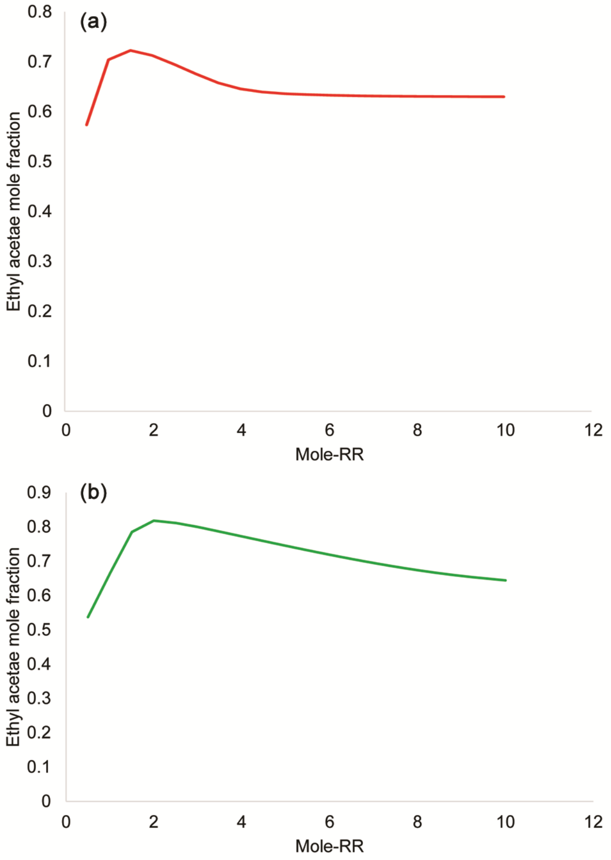

Fig.9 — Effect of mole-RR for (a) rate-based and (b) equilibrium based on ethyl acetate production

Equilibrium model

Fig. 9b, shows reflux ratio effect on mole fraction of EA. From figure, it is observed that as reflux ratio increases the EA formation increases. When it reaches reflux ratio of 2.1, the maximum EA formation is observed. Further increase in reflux ratio causes decrease in formation of EA. The higher reflux ratio, more vapour and liquid contact can occur in the distillation column; thus it increases and it will get highest EA at 2.1. After that as the reflux ratio increases mole fraction of ethyl acetate decreases due insufficient contact of reactant with catalyst surface in the reactive section.

Acid feed stage

Selection of feed stage is the key factor to maintain the more reaction rate in the reactive zone.

Rate based model

The influence of acid feed location on EA mole fraction in distillate versus stage number is shown in Fig. 10a for rate based model. EOH is fed at 14th stage and AA feed location is varied from 4th to 14th stage. It can see that from stage 4th to 9th there is an increase in the ethyl acetate formation and later it is decreasing. From the Fig. 10a, it can see that at 9th stage, the highest mole fraction of ethyl acetate is achieved. The reason for increase in mole fraction of ethyl acetate is maintain of high concentration of reactants in reactive zone.

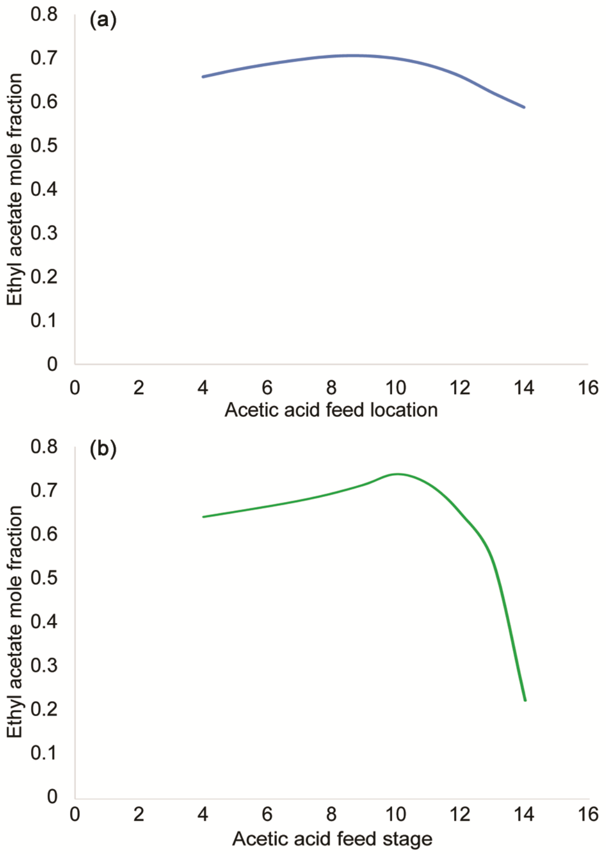

Fig. 10 — Effect of acid feed location on stage for (a) rate based and (b) equilibrium model on ethyl acetate production

Equilibrium model

Fig. 10b shows influence of acetic acid feed location on EA purity in distillate. From the Fig.10b, it is observed that as acid stage location increasing from 4th stage to 10th stage, there is gradual increase in mole fraction of EA because more concentration of reactants in the reactive zone with catalyst surface. Further increase feed location stage number decreases ethyl acetate mole fraction rapidly.

Ethanol feed stage

Rate based model

Further sensitivity analysis has been performed to observe change in EA mole fraction by varying EOH stage as shown in Fig. 11a.The acid feed stage is fixed

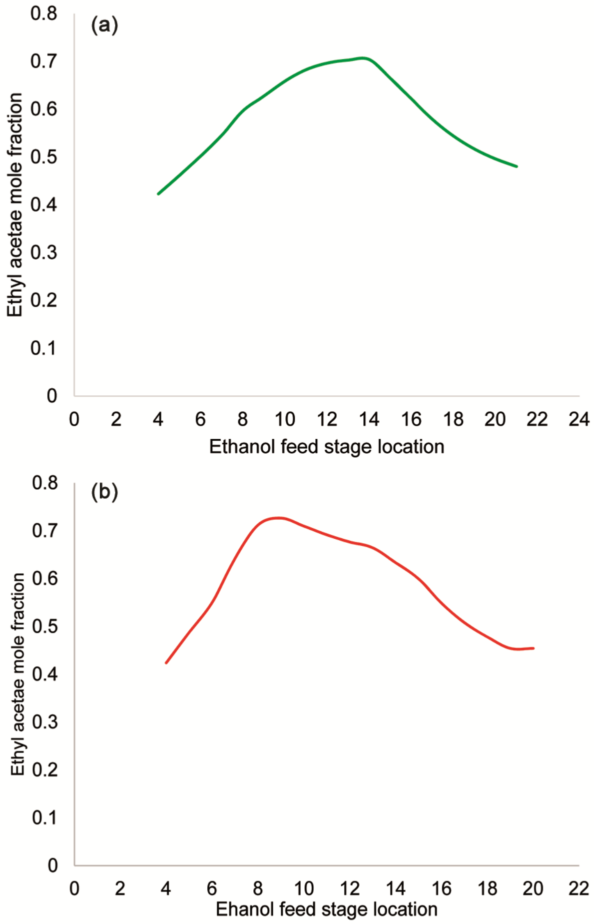

Fig. 11 — Effect of ethanol feed stage for (a) rate based and (b) equilibrium model on ethyl acetate production

and EOH feed stage is changed from 4th- 21rd stage. From Fig. 11a, it can be observed that mole fraction of EA increasing gradually from 4th stage to 14thstage and at 14th stage mole fraction is 0.704. The feed location of EOH at 14th is the optimum stage for maximum EA production. Beyond 14th stage the mole fraction of EA is gradually decreases till 21st stage. The reason is more vapour generation reduces mass transfer between the phases for separation in stripping section.

Equilibrium model

The influence of ethanol feed stage on EA mole fraction is shown in Fig.11b. From the Figure, it is observed that variation of ethanol feed location will influence in EA production. The AA stage is fixed and ethanol feed stage is varied from 4th till 20th stage. It is observed from Fig 11b, that mole fraction of EA increases from 4th to 9th stage. The maximum EA mole fraction has achieved when the feed location of methanol is at 9th stage. Then the mole fraction of EA is decreases from 10th to 15th stages. The reason is more vapour generation reduces mass transfer between the phases for separation in stripping section.

Conclusion

The modelling and simulations have performed for ethyl acetate production in RD column. The comparison of equilibrium and non-equilibrium model based simulations is performed under different parameters for ethyl acetate. The performance of reactive distillation column was simulated under various operating parameters and optimal parameters for high purity ethyl acetate were found for both models. The temperatures and composition profiles with respect to stage number have studied for both models. The sensitivity analysis have performed for mole ratio and feed locations for optimal conditions. From the simulation results it is found that RB model is a better model than equilibrium model. The composition of ethyl acetate is 71.41% from RB model whereas equilibrium model it is 66.45%.

Nomenclature

a	interfacial area (m^2/m^3)
D	distillate flow rate (mol/L)
E	energy hold-up (J/mol)
F	feed composition
h_{tc}	heat transfer coefficient($W/m^2.K$)
H	enthalpy (J/mol)
i	component index
I	inter phase
j	stage index
k	mass transfer coefficient(m/s)
K	equilibrium constant
L	liquid flow rate (mol/L)
L	liquid phase
M	molar hold up (mol)
N	mass flux ($mol/m^2.s$)
r	reaction rate(mol/L.min)
RR	reflux ratio
T	temperature (°C)
V	vapour flow rate (mol/L)
V	vapour phase
U	reaction volume (L)
x	liquid mole fraction
y	vapour mole fraction

Acknowledgement

The author gratefully acknowledges Sun Pharmaceutical Industries Ltd. for sanctioning the

Project (P.O. No. 5000237689) to conduct research on reactive distillation.

Conflict of interest

The author declares no conflict of interest.

References

1 Agreda V H & Partin L R, US Patent, (1984) 4435595.

2 Agreda V H, Partin L R & Heiss W H, High purity methyl acetate via reactive distillation, *Chem Eng Prog*, 86 (1990) 40.

3 Taylor R & Krishna R, Modeling reactive distillation, *Chem Eng Sci*, 55 (2000) 5183.

4 Mekala M, Experimental and simulation studies of a continuous reactive distillation for an esterification process, *Int J Chem React Eng*, 11 (2022) 1193.

5 Lee J H & Dudukovic M P, A comparison of the equilibrium and non-equilibrium models for a multicomponent reactive distillation column, *Comp Chem Eng*, 23 (1998) 159.

6 Alejski K & Duprat F, Dynamic simulation of multicomponent reactive distillation, *Chem Eng Sci*, 51 (1996) 4237.

7 Pöpken T, Steinigeweg S & Gmehling J, Synthesis and hydrolysis of methyl acetate by reactive distillation using structured catalytic packing: Experiments and simulation, *Ind Eng Chem Res*, 40 (2001) 1566.

8 Bessling B, Loning J, Ohligschlager A, Schembecker G & Sundmacher K, Investigation on the synthesis of methyl acetate in a heterogeneous reactive distillation process, *Chem Eng Technol*, 21 (1998) 393.

9 Mallaiah M & Goli V R, Simulation of continuous packed bed reactive distillation column for the esterification process using activity based kinetic model, *Theor Found Chem Eng*, 50 (2006) 404.

10 Sohailrasool L & Syedakhl A, Modeling and simulation of ethyl acetate reactive distillation column using aspen plus, *Int J Eng Res Technol*, 3 (2012) 327.

11 Ruining H , Yun Z , Yanbo D, Yaseen M, Sidra S & Zhangfa T, Kinetic study and process simulation of esterification of acetic acid and ethanol catalyzed by [HSO_3-bmim][HSO_4], *Chem Eng Res Des*, 137 (2018) 235.

12 Abdulwahab G, Saidat O G, İsmail B & Süleyman K, Simulations and economic analyses of ethyl acetate productions by conventional and reactive distillation processes using aspen plus, *Inter J Eng Res Technol*, 2 (2013) 594.

13 Anton A K, Novel catalytic reactive distillation processes for a sustainable chemical industry, *Top Catal*, 62 (2018) 1132.

14 Chavdar C & Evgeni S, Reactive distillation for ethyl acetate production, *J Chem Technol Metall*, 52 (2017) 463.

15 Mayra F F, Benoît B, Xuân-Mi M, Michel M, Marie-Véronique L L, Galo C L R & Mathias B, Experiments and dynamic modeling of a reactive distillation column for the production of ethyl acetate by considering the heterogeneous catalyst pilot complexities, *Chem Eng Res Des*, 91 (2013) 2309.

16 Branislav S, Juraj L & Zuzana L, Multi-aspect comparison of ethyl acetate production pathways: Reactive distillation process integration and intensification via mechanical and chemical approach, *Processes*, 8 (2020) 1618.

17 Santaella M A, Orjuela A & Narváez P C, Comparison of different reactive distillation schemes for ethyl acetate production using sustainability indicators, *Chem Eng Process: Process Intensif*, 96 (2015) 1.

18 Peng J, Lextrait S, Edgar T F & Eldridge R B, A comparison of steady-state equilibrium and rate-based models for packed reactive distillation columns, *Ind Eng Chem Res*, 41 (2002) 2735.

19 Zeki N S A, Al-Hassani M H & Al-Jendeel H, A Kinetic study of esterification reaction, *Al-Khwarizmi Eng J*, 6 (2010) 33.

20 Peng J, Edgar T F & Eldridge R B, Dynamic rate based and equilibrium models for a packed reactive distillation column, *Chem Eng Sci*, 58 (2003) 2671.

21 Taylor R & Krishna R, Multicomponent mass transfer, New York, Wiley (1993).

22 Reddy B, Bhat R, Agrawal A, Patidar P & Mahajani S, Comparison of reactive chromatography and reactive distillation for the synthesis of C1-C4 acetates, *Chem Eng Proc Proc Inten*, 95 (2015) 17.

23 Singh D, Gupta R K & Kumar V, Simulation of a plant scale reactive distillation column for esterification of acetic acid, *Comput Chem Eng*, 73 (2015) 70.