Rate-Based Model In Bubble-Cup Batch Distillation Column

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Abstract

The present work concerned with studying the behavior of batch multicomponent plate distillation tower using Rate-Base model (Non-Equilibrium model) theoretically and experimentally. The experimental work was performed by using a batch distillation column consisting of eight bubble-cup trays. A zeotropic (nonazeotropic) system of Benzene, Toluene, and Ethylbenzene (B-T-EB) has been used. In the experimental work the effect of reflux ratio, heat duty, and initial charge composition on the batch distillation process have been studied. The range of reflux ratio was 1 - 4, heat duty was 222 and 336 Watt, and the initial charge composition was 0.2 - 0.5 mole fraction of the light component (benzene) and for the heavy component (ethylbenzene).

The theoretical work was performed through several steps in order to construct and develop a model based on simultaneous heat and mass transfer between vapor and liquid phases called "Nonequilibrium or Rate-Based model", which is based on **MERSHQ** equations (Material, Energy balances, Rate of mass and heat transfer, Summation of composition Hydrodynamic equation of pressure drop, and eQuilibrium relation

The performance and validity of the developed non-equilibrium-based model gave a good agreement with the experimental work on Benzene-Toluene-EthylBenzene system.

Keywords: Nonequilibrium, Batch Distillation, Trayed Column

النمذجة المعتمدة على معدل انتقال المادة و الطاقة لعمود تقطير الدفعات ذو الصواني الفقاعية

الخلاصة

تم دراسة سلوكية عمود تقطير الدفعات ذو الصواني لخليط متعدد المكونات عمليا و نظريا. الدراسة العملية أنجزت من خلال إجراء التجارب باستخدام عمود لتقطير الدفعات يتألف من ثمان صواني فقاعية تم استخدام نظام اعتيادي (غير ايزوتروبي) مؤلف من البنزين والتلوين والاثيل بنزين الدراسة العملية تضمنت دراسة تأثير نسبة الراجع و الحمل الحراري والتركيب الابتدائي المشحون في إناء الغلاية على عملية التقطير ذو الدفعات نسبة الراجع التي تم دراستها كانت من المشحون في إناء الغلاية على عملية التقطير ذو الدفعات نسبة الراجع التي تم دراستها كانت من المشحون في إناء الغلاية على عملية التقطير ذو الدفعات نسبة الراجع التي تم دراستها كانت من المشحون في الناء الغلاية على عملية التقطير أو الم التركيب الابتدائي المشحون فكان 2.0-5.0 كسر مولي بالنسبة لكل من المادة الخفيفة (البنزين) والمادة الثقيلة الاثيل بنزين) الدراسة النظرية أنجزت من خلال عدة خطوات لغرض إنشاء و تطوير موديل معتمد على أسلوب على عدم التوازن أو (معدل الكتلة والطاقة المترادفة بين الأطوار والتي تدعى "النمذجة المعتمدة على عدم التوازن أو (معدل الجريان)" والتي تعتمد على معادلات معمدة الميزية المادة والطاقة ومعدل جريان المادة والطاقة مع جمع التراكيب وكنك المعادلة الهيدرودينميكية ليهبوط الضغط بالإضافة إلى علاقات التوازن أداء الموديل أعطى توافق جيد الهيدرودينميكية ليهبوط الضغط بالإضافة إلى علاقات التوازن أداء الموديل أمع موالية المعادلة مع النتائج العملية.

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Introduction

One of the major operations in the chemical, petroleum, and pharmaceutical industries is the separation of the liquid mixtures into their components by using distillation.

Batch distillation has the advantage of being much more flexible than continuous distillation. The flexibility makes batch distillation possible to cope with varying compositions of feed and product specifications; also completely different mixtures can be separated with high purity products using the same column^[1].

During the last century the equilibrium- based model had been used to model staged separation operations. Important advances in numerical methods have made equilibrium-stage possible the treatment of complex separation systems with very flexible sets of Although specifications. the equilibrium-based model, modified to incorporate stage efficiency, may be adequate in many cases of binary mixtures, its deficiencies for more general cases and for application to multicomponent mixtures of three or more components have long been recognized. Practical applications of the results by means of stage efficiency have, however, always especially been suspect, for transfer. multicomponent mass Therefore, the development of a more realistic nonequilibrium, transport or rate-based model has long been a desirable goal^[2].

It is now possible to develop and apply a completely nonequilibrium (or

rate)-based model to the calculation of staged separation, which is based on **MERSHQ** equations. The advantages of this approach can usher in a new era for modeling^[2].

In 1977, Waggoner and Loud^[3] developed а rate-based. mass transport model limited to nearly ideal, close-boiling, multicomponent systems. However an energy transport equation was not included (because thermal equilibrium would be closely approximated for close boiling mixture) coupling and the of component mass transfer rates was ignored.

In 1979, Krishna and Standart^[4] showed the possibility of applying rigorous multicomponent mass and heat transfer theory to calculate simultaneous transport. The theory was further developed by Taylor and Krishna, 1993^[5]. The availability of this theory led to development in 1985 by Krishnamurthy and Taylor^[6] of the first general rate-based, computer-aided model for application to trayed and packed columns for distillation and other continuous, countercurrent vapor-liquid separation operations.

In 1985, Krishnamurthy and Taylor^[6] made a comprehensive extension of Sorel's equilibrium-stage model to a nonequilibrium-stage computer algorithm (based on fairly general multicomponent mass and energy transport models). Such a development was а significant accomplishment chemical in The engineering. previous development of algorithms for equilibrium-stage required models

only a sound knowledge of thermodynamics and applied

mathematics; the development of an algorithm for a rate-based model also requires a comprehensive knowledge of the difficult area of coupled multicomponent mass and energy transport.

A nonequilibrium or rate-based model employs a transport phenomena approach and the film model description for predicting the mass transfer rates. It assumes that the equilibrium is established at the interface between vapor and liquid phases. The fluxes of mass and energy across the interfacial area from bulk phase to other. Mass and heat transfer correlations are an integral part of the nonequilibrium model^[7].

Present Work

The present work emphasized to construct a mathematical model based on the new manner of the modeling that called nonequilibrium (or rate)based model, for traved-type multicomponent batch distillation column. The proposed model predict liquid and vapor composition profile, liquid and vapor temperature profile, liquid and vapor internal flow rates, distillate flow rate and composition, stage holdup profile, mass and heat transfer rates between phases. The following assumptions were proposed for the developed model:

- 1. The vapor-liquid interface is at thermodynamic equilibrium.
- 2. The vapor and liquid reached thermodynamic equilibrium on trays just at steady state in total reflux condition.

- 3. The trays are in mechanical equilibrium; $P_j^V = P_j^L = P_j$.
- 4. The mass and energy transport are from vapor phase to liquid phase.
- 5. The flow patterns are plug flow for vapor through perfectly mixed liquid.
- 6. The total molar holdup of vapor and liquid on the tray are constant during any short time interval.
- 7. The condenser operates at total condensation.
- 8. The modeling of reboiler and condenser based on equilibrium model.
- 9. The pressure along the column is constant due to low-pressure drop that had been measured during the experiments.
- 10. The walls of the column are perfectly insulated.

The performance and validity of the developed model were compared with experimental results obtained throughout the present work.

The feed system used in the present work Benzene-Toluene-Ethylbenzene was considered as a wide-boiling point system 80.1, 110.6, 136.1°C respectively, and it is also considered as a zeotropic system (nonazeotropic). This was detected through drawing of the residue curve map of the system, where it was clear that the system is zeotropic^[8]. The predicted equations of the physical properties of the system that used in the model had been tested with some available experimental data ^[8].

The variables studied for this system are reflux ratio, heat duty and the

initial charge composition and they are in the range of 1-4, 220 and 336W and 0.2-0.5 for each light component

(Benzene) and heavy component (Ethylbenzene) respectively.

Experimental Work

The experiments were carried out using a laboratory scale batch distillation column shown as a photograph in Figure (1). The distillation column consists of a still pot, which is heated by using a heating mantle. The column is located above the still pot, and consists of eight bubble-cap trays, each one, 30 cm³ liquid holdup, equipped with sampling valve and thermocouple sensor. At the top of the column, a double-pipe condenser is connected, which is used to condense the vapor leaving the top of the column. Another double-pipe condenser located prior to the distillate collection pot is used to ensure that there is no vapor exit as product and cool the distillate. A magnetic reflux unit (solenoid valve) situated near the top of the column, connected to the interface unit, and through which the reflux ratio is adjusted and controlled. The rate of condensate being sent to 2-liter graduated glass vessel for distillate collection. The outlets of the second condenser and the collecting vessel are provided with sampling valves.

The main column 1 m height and 8.1 cm inner diameter is connected at the lower part to a 2 liters capacity spherical heat resistant glass vessel with four open necks for installing instruments, as well as a sampling valve. The still pot is equipped with 500-Watt electrical heating mantle. The electrical heater power is regulated by an interface unit connected to a personal computer.

The experimental work was performed by measuring the temperatures in reboiler, trays, and condenser, the composition at various locations along the column, and the column pressure drop. The analyses of the samples were carried out using GC of type PYE UNICAM (series-204). instrumented with Flame Ionization Detector (FID).

The experimental data, which are collected during present study, consisted of the measurement of the temperature for all stages and of the compositions of reboiler, tray-No.5 (optional selected), and condenser. These data are used to evaluate the performance of the developed nonequilibrium-based model.

The operating conditions that has been studied in the present work are given in table (1).

Experiments 1, 2, and 3 in table (1) are for studying the effect of reflux ratio. In these experiments three different values for reflux ratio (R = 1, 2, and 4) are chosen. Experiments number 3, and 4 were conducted to study the effect of changing the heat duty supplied to the still. And the experiments number 3, 5, and 6 were conducted, each one, with different charge composition in the still but constant reflux ratio and heat duty. All these experiments are carried out in order to get various of compositions responses and temperatures along the distillation column and compare them with the

results that are predicted from the developed nonequilibrium model. All experimental data that extracted in this study are available^[8].

Theoretical Nonequilibrium Model

Theoretical model for Nonequilibrium stage consider a batch (unsteady state) multicomponent distillation column consisting of a number of stages arranged counter currently. Figure (2) shows the outline for the batch distillation column with nonequilibrium model. The starting point of stage numbering begins from the bottom to the top.

<u>The Nonequilibrium-Stage Model</u> <u>Equations for Tray-j:</u>

The outline of the proposed stage j Figure (2) at which the assumption was that the fluid is split into two distinct phases one for vapor and the other for liquid, and the mathematical analysis was based on each phase separately.

<u>M</u>. Total and component Material balances

The total material balances for vapor and liquid phases are:

$$\frac{dM_{j}^{v}}{dt} = V_{j-1} - V_{j} - N_{T,j}$$
(1)

$$\frac{dM_{j}^{L}}{dt} = L_{j+1} - L_{j} + N_{T,j}$$
(2)

The amount of liquid staying on a tray is the holdup. The liquid hold up is a function of the geometry and the type of contacting device; therefore the liquid volumetric holdup is often constant^[9]. As the liquid volumetric holdup is constant the remaining space that occupied by the vapor is constant too, i.e. the volumetric holdups of the liquid and vapor are constant on a tray.

In fact the change in molar density does not vary considerably on any tray during short intervals of time.

Thus, during short intervals of time,
$$\frac{dM_j^V}{dt} \approx \frac{dM_j^L}{dt} \approx 0...(3)$$

Then,

$$V_{j} = V_{j-1} - N_{T,j}$$
 j=2,3,...,(N-1)
.....(4)
 $L_{j+1} = L_{j} - N_{T,j}$ j=2,3,...,(N-1)
....(5)

The component material balance of component i in vapor and liquid phases on stage j are:

$$\frac{dy_{i,j}}{dt} = \frac{V_{j-1}}{M_j^V} y_{i,j-1} - \frac{V_j}{M_j^V} y_{i,j} - \frac{N_{i,j}^V}{M_j^V}$$

$$\frac{dx_{i,j}}{dt} = \frac{L_{j+1}}{M_j^L} x_{i,j+1} - \frac{L_j}{M_j^L} x_{i,j} + \frac{N_{i,j}^L}{M_j^L}$$
....(7)

<u>E</u>. Energy balances

The energy balances of vapor and liquid phases on stage j are:

$$\frac{dH_{j}}{dt} = \frac{V_{j-1}}{M_{j}^{V}}H_{j-1} - \frac{V_{j}}{M_{j}^{V}}H_{j} - \frac{e_{j}^{V}}{M_{j}^{V}} (8)$$
$$\frac{dh_{j}}{dt} = \frac{L_{j+1}}{M_{j}^{L}}h_{j+1} - \frac{L_{j}}{M_{j}^{L}}h_{j} + \frac{e_{j}^{L}}{M_{j}^{L}} (9)$$

<u>R</u>. Rate of mass and energy across the interface

At the vapor-liquid interface, there is no mass or energy accumulation. Thus,

$$N_{i,j}^{V} = N_{i,j}^{L}$$
 (10)

$$\boldsymbol{e}_{j}^{V} = \boldsymbol{e}_{j}^{L} \tag{11}$$

<u>S</u>. Summation of mole fractions

Summation of the mole fractions at vapor-liquid interface are:

$$\sum_{i=1}^{C} y_{i,j}^{I} = 1.0$$
(12)

$$\sum_{i=1}^{\infty} x_{i,j}^{I} = 1.0 \tag{13}$$

and the normalization procedure that are used in equilibrium-stage model^[10] will be used for mole fractions of vapor and liquid phases in present nonequilibrium-based model. Thus,

$$(y_{i,j})_{normalized} = \frac{y_{i,j}}{\sum_{i=1}^{C} y_{i,j}}$$
 (14)

$$(x_{i,j})_{normalized} = \frac{x_{i,j}}{\sum_{i=1}^{C} x_{i,j}}$$
 (15)

<u>H</u>. Hydraulic equation of pressure drops

The distillation column operates at atmospheric pressure. The condenser pressure is equal to atmospheric pressure, and the pressure in the reboiler is slightly higher than the condenser by the amount equal to the measured pressure drop. The measured pressure drop along the column was between 600Pa maximum and 550 Pa minimum. This means that the average pressure drop was 575Pa, which is small enough to consider the column to be operated at constant pressure.

<u>Q.</u> eQuilibrium equation at vapor-liquid interface

The thermodynamic equilibrium of each component was assumed to exist only at the interface:

$$y_{i,j}^{I} = K_{i,j} x_{i,j}^{I}$$
(16)

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<u>The Nonequilibrium-Stage Model</u> Parameters of Tray-j:

1. Rate of mass and energy transport calculation

The rate of component mass transfer across the vapor and liquid

films was based on the consideration of diffusive and convective (bulk-flow) contributions. Thus,

$$(N_{i,j}^{v}) = (J_{i,j}^{v}) + (\overline{y}_{i,j})N_{T,j} \quad (17)$$

$$(N_{i,j}^{L}) = (J_{i,j}^{L}) + (x_{i,j})N_{T,j} \quad (18)$$

$$(J_{i,j}^{v}) = c_{T}^{v}[ka_{i,j}^{v}]A(\overline{y}_{i,j} - y_{i,j}^{l}) \quad (19)$$

$$(J_{i,j}^{L}) = c_{T}^{L}[ka_{i,j}^{L}]A(x_{i,j}^{l} - x_{i,j}) \quad (20)$$

$$\sum_{i=1}^{C} N_{i,j}^{v} = \sum_{i=1}^{C} N_{i,j}^{L} = N_{T,j} \quad (21)$$

where, $\hat{J}_{i,j}^{P} = AaJ_{i,j}^{P}$, *P* represent vapor or liquid phase. The total flux on tray-j, $N_{T,j}$ across the interface needed in these equations was obtained from the summation equation at the interface, that is the interface mole fractions were iterated until the mass transfer fluxes were equal at both sides of the interface and the sum of the interface mole fractions is unity^[11].

Many models^[12,13,14] were available for prediction of binary pair mass transfer coefficient and interfacial area. The predicted values of Grester et al. model^[13] were the most appropriate as compared with those of the other models for the present work. Therefore this model has been chosen to evaluate the product of binary pair mass transfer coefficient and interfacial area $k_{ik}^{P}a$. This model used only for bubble-cap trays.

The determination of values of $[k_{ik}^{P}a]$ are from reciprocal mass-transfer coefficient function^[4] of vapor and liquid phases mixtures. Thus, for a nonideal gas mixture: $[k^{V}] = [R^{V}]^{-1}[\Gamma^{V}]$ (22) And for a nonideal liquid mixture: $[k^{L}] = [R^{L}]^{-1}[\Gamma^{L}]$ (23)

The term $[\Gamma^{P}]$ in these equations can be ignored where, for nonideal vapor, $a[\Gamma^{V}]$ term is rarely necessary^[10].

The elements of \hat{R} (in terms of the product of mass transfer coefficient and interfacial area ka_{ik}) is:

$$\begin{pmatrix}
\mathbf{R}_{ii} = \frac{z_i}{\mathbf{k}a_{iC}} + \sum_{\substack{k=1\\k\neq i}}^{C} \frac{z_k}{\mathbf{k}a_{ik}} \quad (24) \\
\begin{pmatrix}
\mathbf{R}_{ik} = -z_i \left(\frac{1}{\mathbf{k}a_{ik}} - \frac{1}{\mathbf{k}a_{iC}}\right) \quad (25)
\end{pmatrix}$$

The rate of energy transfer across the vapor and liquid films is based on the sum of the convective heat transfer and the products of enthalpies times the mass transfer contributions:

$$e_{j}^{v} = h_{i}a^{v}(T^{v} - T^{T}) + \sum_{i=1}^{L}N_{i,j}\overline{H}_{i,j}$$

...(26)
$$e_{j}^{L} = h_{i}a^{L}(T^{T} - T^{L}) + \sum_{i=1}^{C}N_{i,j}\overline{h}_{i,j}$$

...(27)

Heat transfer coefficients for the vapor film are estimated from the Chilton-Colburn analogy between heat and mass transfer and for the liquid phase film, a penetration model is preferred^[10]. Thus $h_{i}a^{v} = ka^{v} r^{v}Cp^{v}(Le^{v})^{2/3}$ (28)

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$$h_{t}a^{L} = ka^{L} r^{L} Cp^{L} (Le^{L})^{1/2}$$
(29)

2. Total holdup calculation:

The model was based on constant molar holdup on trays during short intervals of time; therefore the vapor and liquid molar holdups on tray j were evaluated periodically through:

$$M_{j}^{V} = \frac{\text{Vap. Vol. on tray}}{\sum_{i=1}^{C} \frac{y_{i} M w t_{i}}{r_{i}^{V}}}$$
(30)
Liq. Vol. on tray

$$M_{j}^{L} = \frac{\text{Liq. Vol. on tray}}{\sum_{i=1}^{C} \frac{x_{i} M w t_{i}}{r_{i}^{L}}}$$
(31)

3. Enthalpy calculation

The enthalpy of vapor and liquid phases mixtures were calculated by using the following two equations:

$$H_{j} = \sum_{i=1}^{C} y_{i,j} H_{i,j}$$
(32)

$$h_{j} = \sum_{i=1}^{C} x_{i,j} h_{i,j}$$
(33)

The heats of mixing were ignored in the present study. For gases, the heats of mixing are usually negligible^[15].

4. Equilibrium relation calculation

At the vapor-liquid interface, a thermodynamic equilibrium is assumed to be established and the following relation relates the composition of component in vapor phase with the composition of component in liquid phase on tray j: $y_{i,i}^{I} = K_{i,i}x_{i,i}^{I}$ (34)

where,

$$K_{i,j} = \frac{P_{i,j}^{\bullet}}{P} \frac{g_{i,j}}{f_{i,j}^{V}}$$
(35)

where, $P_{i,j}^{\bullet}$ is the vapor pressure of component i on tray j and its value is function of temperature and component constant parameters according to Antoine's equation that used to evaluate the vapor pressure values.

UNIQUAC model have been used to evaluate the activity coefficient for liquid phase $g_{i,j}$. UNIQUAQ model gives the best prediction value (minimum deviation error) with respect to experimental data than the other models^[8].

For evaluating of the component fugacity coefficient in the vapor phase $f_{i,j}^{V}$, two models had been compared, (Virial equation, and Redlich/Kwong equation). Virial equation is implemented in the present modeling sense the values that have been predicted form these two models are very close and they are rarely, below $0.95^{[8]}$.

5. Flow Patterns

The evaluations of driving forces of mass transport and energy transport are strongly depending on the flow patterns chosen for the vapor and liquid phases.

In the present simulation of laboratory-scale tray column, a plug vapor flow pattern was assumed by using the arithmetic average composition for the vapor phase (the logarithmic average gives virtually identical results) and a perfectly mixed liquid flow pattern was

assumed by using the outlet liquid composition as liquid bulk composition^[6].

The Reboiler Model

The well-known **MESH** equations are used for modeling the reboiler

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Figure (3), where the total material balance is:

$$\frac{dM_{\rm f}^{\rm f}}{dt} = L_2 - V_1 \approx \frac{\Delta M_1^{\rm f}}{\Delta t} \approx \frac{M_1^{\rm f}(t + \Delta t) - M_1^{\rm f}(t)}{\Delta t} \dots (36)$$

where, M_1^L is the total liquid holdup, whose quantity decreases continuously during the production period of the batch operation.

The variation of the total liquid molar holdup in the reboiler is:

$$M_1^L(t) = M_1^0 - \sum_{j=2}^{10} M_j^L - \sum_{j=2}^{9} M_j^V - \int_0^t Ddt..(37)$$

where M_1° is the initial charge to the still.

A component material balance is:

$$\frac{dx_{i,1}}{dt} = \frac{L_2}{M_1^L} x_{i,2} - \left(\frac{L_2 + V_1(K_{i,1} - 1)}{M_1^L}\right) x_{i,1} \dots (38)$$

The energy balance is:

$$\frac{dh_1}{dt} = \frac{L_2}{M_1^L} (h_2 - h_1) - \frac{V_1}{M_1^L} I_1 + \frac{Q_B}{M_1^L} A..(39)$$

Rearrangement of equation (39) gives:

$$V_{1} = \frac{\frac{\Delta M_{1}^{L}}{\Delta t}(h_{2} - h_{1}) + Q_{B} - M_{1}^{L}\frac{\Delta h_{1}}{\Delta t}}{I_{1} - (h_{2} - h_{1})} \dots (40)$$

where,
$$l_1 = H_1 - h_1$$
, and
 $\frac{dh_1}{dt} \approx \frac{\Delta h_1}{\Delta t} \approx \frac{h_1(t + \Delta t) - h_1(t)}{\Delta t}$ (41)

Summation equations for vapor and liquid phases are also considered. Thus,

$$\sum_{i=1}^{C} x_{i,1} = 1 \text{ and } \sum_{i=1}^{C} y_{i,1} = 1$$
 (42)

The Condenser Model

The condenser is operated at total condensation Figure (3). Total and component material balances are:

$$\frac{dM_{C}^{L}}{dt} = V_{9} - (L_{C} + B) \approx \frac{DM_{C}^{L}}{Dt}$$
(43)

where, M_C^L is the total liquid holdup, and B_C is the distillate.

A component material balance is:

$$\frac{dx_{i,C}}{dt} = \frac{V_9}{M_{10}^L} (y_{i,9} - x_{i,D}) \quad (44)$$

From the energy balance:

$$\boldsymbol{Q}_{C} = \boldsymbol{V}_{9} \boldsymbol{1}_{C} - \boldsymbol{M}_{C}^{L} \frac{\boldsymbol{D}\boldsymbol{h}_{C}}{\boldsymbol{D}\boldsymbol{t}}$$
(45)

where, $\mathbf{l}_{c} = \mathbf{H}_{9} - \mathbf{h}_{c}$ The liquid in the condenser is saturated liquid i.e. the liquid at bubble point temperature of its mixture. Thus;

$$\sum_{i=1}^{L} K_{i,D} x_{i,D} = 1$$
 (46)

The batch distillation column was operating at a constant reflux ratio, so that the reflux ratio R is in advance specified variable. Where,

$$R = \frac{L_{10}}{B^2} \tag{47}$$

Results and Discussion

In this section the experimental data obtained from the present study were compared with the simulation results predicted from the developed nonequilibrium model of batch distillation for B-T-EB system.

Figures (4) to (6) show the experimental and simulation results of the compositions profiles (still, tray-5, and distillate) with time for three experiments that had been carried out in the present work. The predictions of components compositions have

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some specialty where, any failure in the prediction of the composition of any component imposes a failure in the prediction of the other compositions because of the restriction to unity. Figures (4) to (6) show a good agreement between the experimental and predicted results. However it is clear from these figures that the results of the nonequilibriumbased model were often overestimated for the benzene composition, and this to an underestimation led for ethylbenzene. This may be due to the high volatilities for all components especially for benzene. The overestimation of the benzene composition is very clear in distillate where, the composition of benzene is the highest.

Figure (7) shows a comparison between the experimental and simulation results for each component, for all experiments, the deviations were bounded by the lines $\pm 20\%$. Also, it is clear from these figures that the model overpredicts the benzene composition, while underpredicts the composition of ethvlbenzene.

Figure (8) gives an overall view for the predictions of the nonequilibrium-based model for the compositions of benzene, toluene, and ethylbenzene at three locations still, tray-5, and distillate as compared with the experimental results Figures (9) to (11) show a comparison between the

experimental and predicted results of temperatures at different stages along the column, the deviations were bounded by the lines $\pm 10\%$.

Conclusion

The conclusions that extracted from the present study have been

listed below for ordinary batch distillation of B-T-EB system:

- 1- The UNIQUAC model for activity coefficient in liquid phase is the most appropriate model for (B-T-EB) system.
- 2- Stiffness ratio in the modeling of the nonequilibrium-stage is higher than that of the equilibrium-stage.
- 3- The low reflux ratio leads to faster separation of the lightest components in mixture, while the high reflux ratio leads to more efficient separation of the lightest component.
- 4- The evident effect of heat duty was on the time of the production period, where the operation of the batch distillation required more time with low heat duty and vice versa.
- 5- The initial charge compositions of a zeotropic system affect the composition distribution along the column and the time required for the complete separation of the lightest components.

References

- [1] Klingberg, Anna, "Modeling and Optimization of Batch Distillation", MSc thesis, Department of Automatic Control, Lund Institute of Technology, Sweden, 2000.
- [2] Seader, J.D., "The Rate-Based Approach for Modeling Stage Separations", Chem. Eng. Prog., 85, 41-49, (1989).
- [3] Waggoner, R.C., and G.D. Loud, Comput. Chem. Engng., 1, 49 (1977).
- [4] Krishna, R., and G.L. Standart, "Mass and Energy Transfer in

Multicomponent Systems", Chem. Eng. Comm., 3, 201 (1979).

- [5] Taylor, R., and R. Krishna, "Multicomponent Mass Transfer", John Wiley and Sons, New York (1993).
- [6] Krishnamurthy, R., and R. Taylor,
 "A Nonequilibrium Stage Model for Multicomponent Separation Processes. Part I: Model Description and Method of Solution", AIChE J., 31, 449, 456, (1985).
- [7] Serrano, S.V.B., "Computer Simulation Studies for the Prodyction of 7-Tetradecene by Reactve Distillation", Master thesis, University of Mississippi State, USA, (2003).
- [8] Ibrahim, Salah S., "Rate-Based model in bubble-cup batch distillation column", PhD Thesis, University of Technology, Chem. Eng. Dep., IRAQ, (2007).
- [9] Galindez, H. and AA Fredenslund, "Simulation of Multicomponent Batch Distillation pocesses", Comput. Chem. Engng., 12, 281 (1988).
- [10] Seader, J.D. and, E.J. Henley, "Separation Process Principles", John Wiley & Sons, Inc New York (1998).
- [11] Alopaeus, V. and J. Aittamaa, "Appropriate Simplification in Calculation of Mass Transfer in a Multicomponent Rate-Based
- [12] Distillation Tray Model", Ind. Eng. Chem. Res., 39, 4336-4345, (2000).

- [13] AIChE, Bubble Tray Design Manual: Prediction of Fractionation Efficiency, New York, (1958).
- [14] Grester, J.A., Hill,A.B., Hochgraf, N.N., and Robinson, D.G., "Tray Efficiencies in Distillation Columns", AIChE Report, (1958).
- [15] Hughmark, G.A. "Models for Vapour Phase and Liquid Phase

Rate Bsed Model in Bubble-Cup Batch Distillaion column

- Mass Transfer on Distillation Trays", AIChE J., Vol. 17, No. 6 p. 1295 (1971).
- [16] Coulson, J.M. and J.F. Richardson, "Chemical Engineering", Pergamon Vol.6 (1985).

Table (1): The Studied Operating	Conditions for the	he Present	Experimental
	Work.		

EXP. Syste No. Set	System	Initial Still Composition (mole fraction)			Reflux	Heat Duty
	Set	Benzene	Toluene	Ethylbenzene	Ratio	(Watt)
1	Set-1	0.3	0.4	0.3	1	336
2	Set-1	0.3	0.4	0.3	2	336
3	Set-1	0.3	0.4	0.3	4	336
4	Set-1	0.3	0.4	0.3	4	222
5	Set-2	0.2	0.3	0.5	4	336
6	Set-3	0.5	0.3	0.2	4	336



Figure (1): Photograph for The Experimental Rig of Batch Distillation Column.



Figure (2): Batch Distillation Column with Nonequilibrium-based Model.



Figure (3): The Configuration of Reboiler with First Tray and condenser with last tray.



Figure (4): Experimental and simulation composition profile for Set-1 (0.3-0.4-0.3 mole fraction of B-T-EB), R=1, Q=336 W. (Points = Exp., Lines = NEQ-Model)



Figure (5): Experimental and simulation composition profile for Set-1 (0.3-0.4 0.3 mole fraction of B-T-EB), R=2, Q=336 W. (Points = Exp., Lines = NEQ-Model)

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Figure (6): Experimental and simulation composition profile for Set-1 (0.3-0.4-0.3 mole fraction of B-T-EB), R=4, Q=336 W. (Points = Exp., Lines = NEQ-Model)



Figure (7): Comparison between experimental and predicted mole fractions for benzene, toluene, and ethylbenzene in still, tray-5, distillate.



Figure (8): Comparison between the experimental and predicted mole fractions for B-T-EB at still, tray-5, and distillate.



Figure (9): Comparison between the experimental and predicted temperature at still.



Figure (10): Comparison between the experimental and



predicted temperature at tray number 5.

Figure (11): Comparison between the experimental and

predicted temperature at condenser.