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Sequential simulation of packed distillation columns using rate-based model

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Abstract−Though a packed column has continuous internal structure from top to bottom, the design procedure of the column handles it like the trayed column in both the equilibrium-stage design and the rate-based model design. The differential equation of material balance is good for the continuous phase of the packed column. But the counter flow of vapor and liquid streams makes solving the differential equation difficult. We propose a sequential solving procedure of the packed-column model using an iterative computation. The computed results for the systems of methanol/ethanol, ethanol/*n*-propanol and methanol/*n*-propanol were compared with the experimental results to examine the usefulness of the proposed procedure for the simulation of the packed column. The comparison indicates that the proposed procedure predicts satisfactory results of column profiles in the packed column.

Keywords: Packed Distillation Column, Rate-based Model, Distillation Simulation

INTRODUCTION

Distillation is well established in terms of process design and operation, because it has long, proven history of design and operation. Though special distillations, such as reactive and azeotropic, are known to be difficult to design, common distillation is readily designed with commercial design programs. Moreover, the graphical design procedures, the McCabe-Thiele method and the Ponchon-Savarit method, have been proven to be good for the approximate design of binary distillation columns [1]. Most of the design and simulation procedures of the distillation utilize equilibrium-stage methods for trayed columns.

Packed columns are widely utilized in the distillation processes due to low pressure drop giving higher distillation efficiency compared with the trayed columns, though their column diameter is limited. They are also good for the complex distillation [2]. The internal structure of the packed column is quite different from that of the trayed column, but the design of the packed column utilizes the design procedure of the trayed column. The height equivalent to a theoretical plate (HETP) gives the necessary height of the packed column for the designed tray number, but the HETP has no theoretical basis [1].

The rate-based model [3,4] also uses the notion of the trayed column in the formulation of system equations, a set of simultaneous equations composed of material and energy balances with the interface equilibrium relation. The model has been used for complex distillation [5]. In the model the composition of vapor leaving a tray is not in equilibrium with the liquid composition at the tray, while the two are in equilibrium in the equilibrium-stage method. Because the equilibrium-stage method sequentially gives the solution in tray-by-tray manner, the computation of tray compositions is straightforward from top to bottom. On the other hand, solving the rate-based model having one large model of the whole column requires iterative computation for a large size of matrix with a proper set of the initial solutions. For the reduction of the matrix size, a reduced rate-based model was introduced by Bonilla et al. [6].

Intrinsically the continuous, homogeneous structure of the packed column is different from that of the trayed column, and none of the above models for the trays represent the process of mass transfer in the packed column properly. In other words, the material balance of the differential equation in the axial direction of the column can demonstrate the packed column the best as presented in Seok and Hwang [7]. In the study we used a horizontal distillation column, and obtained the concentration profile in the column from the vapor phase material balance. Any solution technique of the first-order ordinary differential equation can be applied for the computation of the packed column. However, solving a differential equation derived from the rate-based model of the packed column is difficult, because the vapor and liquid streams flow in countercurrent, leaving unknown boundary conditions for the equation in a section of the column. Unless the whole column makes one model, a sequential computation of the column profile is not possible. Separately, the hydraulics of the packed column was studied using computational fluid dynamic models [8].

In this study we propose a new rate-based model for the packed column simulation, and present its solving procedure of the sequential computation in detail. The computed concentration profile from the proposed model is compared with the experimental results in the methanol/ethanol, ethanol/*n*-propanol and methanol/*n*-propanol systems for the performance evaluation of the model.

MATHEMATICAL MODEL

A typical distillation column with packing is shown in Fig. 1. For the simplicity of modeling, the following assumptions are given.

- The bulk compositions of liquid and vapor are constant for the differential height.
- The compositions of liquid and vapor at the interface are in

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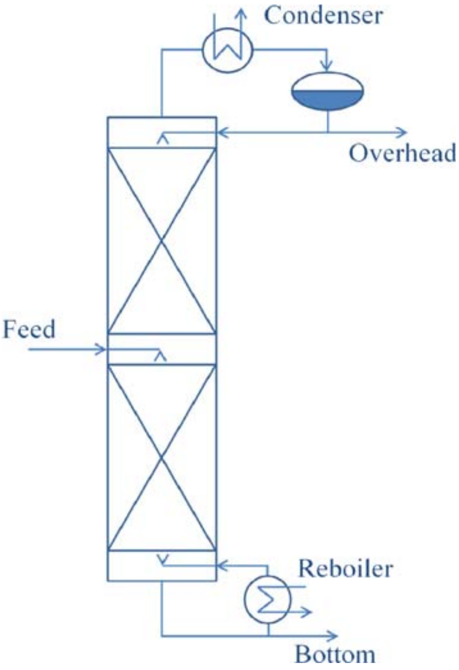

Fig. 1. Schematic diagram of a packed distillation column.

equilibrium.

- The heat of mixing is negligible.
- The axial dispersion of mass and heat is ignored.
- The heat of vaporization and molar enthalpy are constant.

The first and second assumptions are commonly used in the rate-based model [4,7]. The third and last assumptions are related to the energy balance, which is not significant in the adiabatic operation of distillation column. When the vapor and liquid flows are sufficient, the axial dispersion is so small that it can be ignored.

The material balance of light component in the vapor phase for a differential height is formulated as

$$\frac{d(Gy)}{dz}=J_G \tag{1}$$

where the rate of mass transfer through the vapor-liquid interface is

$$J_G=k_G aAc_t^G(y_e-y) \tag{2}$$

The volumetric mass transfer coefficient $k_G a$ in vapor phase is obtained from Billet and Schultes [9], and is listed in Table 1. The parameter A is the cross-sectional area of the distillation column, and

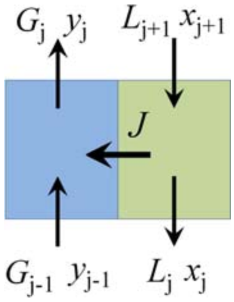

Fig. 2. Description of a rate-based model for the differential height of column.

c_t^G is the concentration of the light component in vapor phase. Fig. 2 demonstrates the mass transfer between the phases for a given height of the column.

Similarly, the material balance in liquid phase is

$$\frac{d(Lx)}{dz}=J_L \tag{3}$$

and the rate of mass transfer in the phase is

$$J_L=k_L aAc_t^L(x_e-x) \tag{4}$$

The total material balance for the differential height

$$\frac{dG}{dz}=-\frac{dL}{dz} \tag{5}$$

and from the component material balance

$$\frac{d(Gy)}{dz}=-\frac{d(Lx)}{dz} \tag{6}$$

The equilibrium relation at the interface is [3,4]

$$y_e=Kx_e \tag{7}$$

The equilibrium constant was calculated from the average relative volatility listed in Table 1. For the examination of the simulation results from the rate-based model of this study, the experimental parameters given in Table 1 are obtained from the references [9,10].

COMPUTAIONAL PROCEDURE

The column size used in this study was adopted from the experiment of Rejl et al. [10], and a 15 cm of diameter and 210 cm of column length were provided in the computation. The structured pack-

Table 1. Parameters used in the model are from the references [9,10]. Two values of flow rates and volumetric mass transfer coefficients indicate two different operating conditions. Relative volatility was calculated from the equilibrium compositions

System	Methanol-ethanol	Ethanol-propanol	Methanol-propanol
Relative volatility	1.69	2.13	3.64
L (m/h)	2.97/11.9	3.67/14.7	3.33/13.3
G (m/s)	0.43/1.71	0.41/1.64	0.41/1.64
C_t^L ($\times10^{-4}$ mol/m^3)	1.83	1.36	1.53
C_t^G (mol/m^3)	35.3	33.8	34.6
$k_L a$ (1/s)	0.01/0.025	0.01/0.026	0.01/0.028
$k_G a$ (1/s)	1.7/7.9	1.6/7.5	1.99/7.1

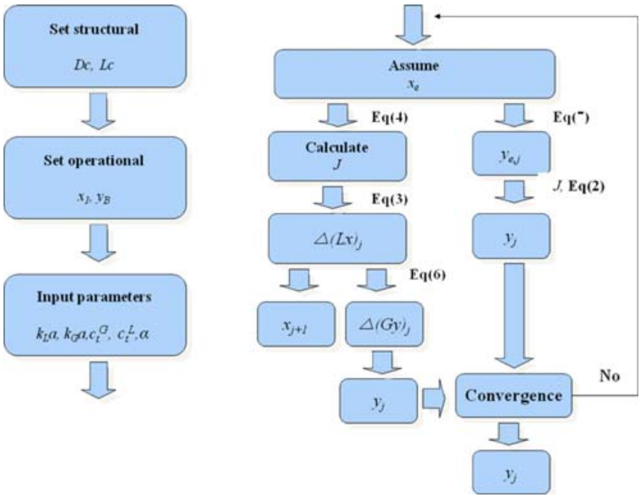

Fig. 3. Algorithm of the computational procedure of liquid and vapor compositions in the differential height of column.

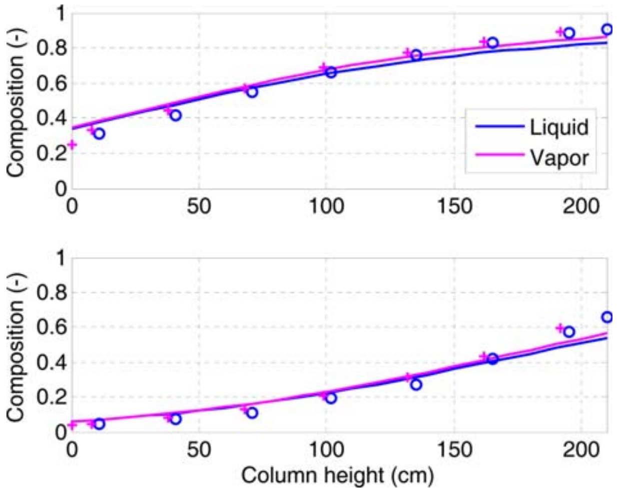

Fig. 4. Liquid and vapor compositions computed from the model compared with the symbols of experimental results for the methanol/ethanol system. Top is of the high rate of liquid flow, and bottom is of low rate.

ing named Mellapak 250Y was used, and its HETP was 33 cm [10]. The liquid composition to the bottom of the column and the vapor composition at the bottom were adjusted for the compositions at the top of the column. These are like the boundary conditions of the material balance. Because the experiment was conducted at total reflux condition, no feed and product was included in the simulation. Other operating parameters are found from the experimental variables and listed in Table 1. Two operating conditions, liquid and vapor flow rates, were presented for each of three alcohol systems of methanol/ethanol, ethanol/*n*-propanol, and methanol/*n*-propanol mixtures. The computation was conducted with MATLAB using home-made code.

When the parameters are set, the vapor composition of light component is calculated from the assumed liquid composition at the interface by two different ways as shown in Fig. 3: one from the mass transfer rate and material balance in liquid, and the other from the equilibrium relation at the vapor-liquid interface and the mass transfer rate across the interface. If the difference of these two vapor compositions is larger than the given value, the assumed liquid composition is revised until their difference reaches the value. The limit was 0.0001 in this study. In the revision of the assumed liquid composition, a portion of the difference was added to the old liquid composition. The computation began at the bottom of the column with the adjusted bottom composition referenced to the composition of bottom product. The calculated composition is of the given height of the column from the bottom, and the computation sequentially continued until it reached the top. The subscript j used in Fig. 2 indicates the number of computation sequence. The differential height was 1 cm in this study.

RESULTS AND DISCUSSION

Though the packed column has quite different internal structure from the trayed column, the computation of its liquid composition inside the column utilizes the scheme of the trayed column in both the equilibrium-stage method and the rate-based model. The packed column has more like a continuous phase inside the column, and the mass transfer between the vapor and liquid phases can be described with a differential volume in the column as the material balance (Eq. (1)). However, the equation is not solved without the liquid composition from the above. To avoid the problem, an iterative procedure is used in this study. A similar procedure was applied in the computation of diabatic horizontal distillation column [11]. The computation results are explained below with the performance evaluation.

1. Computation Results

For the performance evaluation of the proposed simulation procedure, the experimental results of vapor and liquid composition in the packed column were used here. Table 1 lists the operating conditions of the experiment [10]. Fig. 4 demonstrates the computation results in curves with the experimental values in symbols for the methanol/ethanol system. The top figure shows the compositions of vapor and liquid along the column height at high liquid flow rate indicated in Table 1. The bottom one illustrates those of low liquid flow rate. The composition of vapor and liquid at the same column height does not show large difference, especially in the middle of the column. It is explained in the next section. The calculated composition shows relatively good agreement with the experimental results [10], which indicates that the proposed computation procedure using the rate-based model is suitable to simulate the packed distillation column. The component material balance, Eq. (6), indicates that the variation of vapor composition is close to the variation of liquid composition, when the vapor and liquid flow rates are not quite different. Note that the flow directions of vapor and liquid are opposite and the signs are different. The curves of vapor and liquid compositions in Fig. 4 show similar variation as predicted from the material balance. The experimental results [10] demonstrate the close variation. The volumetric mass transfer coefficients used here are adopted from Billet and Schultes [9], but they are not consistent with other empirical prediction models. When the difference of the coefficients found from different experiments and experimental error in the reference [9] are considered, the computed results of this study show good agreement with the experimental outcome [10]. Note that the curve is computed sequentially from the bottom of

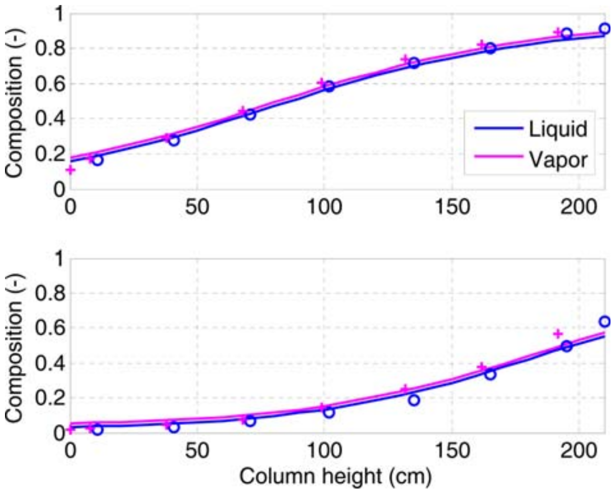

Fig. 5. Liquid and vapor compositions computed from the model compared with the symbols of experimental results for the ethanol/*n*-propanol system. Top is of the high rate of liquid flow, and bottom is of low rate.

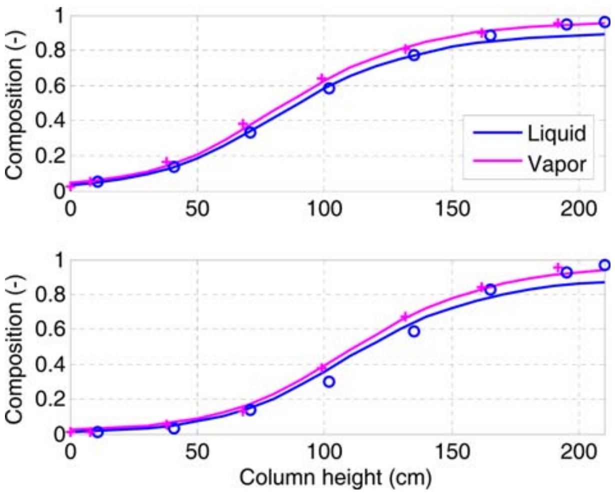

Fig. 6. Liquid and vapor compositions computed from the model compared with the symbols of experimental results for the methanol/*n*-propanol system. Top is of the high rate of liquid flow, and bottom is of low rate.

the column. Therefore, some large gap at the top is from the cumulated errors from the sequential computation. The curve is not fitted to the experimental results of the symbols.

Fig. 5 demonstrates the results of ethanol/*n*-propanol system. The computed curve is closer to the experimental results than the methanol/ethanol system [10]. The top figure is of the high liquid flow listed in Table 1, and the bottom is of low flow rate. Finally, the results of the methanol/*n*-propanol are shown in Fig. 6. Similar difference between the computed and experimental results to other systems is obtained.

2. Modeling Errors

In the calculation of mass transfer rate Eqs. (2) and (4), the role of convective flow was not accounted by assuming equimolar counter diffusion [10]. This is widely used in distillation column design, such as the graphical procedure. The variation of liquid and vapor flow rates through the same section of the column is small. When the liquid flow rates were computed from the rigorous simulation of methanol/ethanol system with 20 trays using the HYSYS, the calculated variation of the liquid flow was 4.3% in the rectifying section top to bottom. Therefore, the effect of the equimolar assumption in the composition comparison is not significant in this study. The elimination of energy balances in the proposed model is due to the assumption of equimolar counter diffusion.

More difference at the high column height as demonstrated in Figs. 5 and 6 is from the cumulative computation error, because the computation is sequentially carried out from the bottom. In the equilibrium-stage calculation method, the gap between liquid and vapor phase compositions is large in the middle of the column, but the large middle gap is not shown in the results of this study. The experimental results do not indicate the gap either except the methanol/*n*-propanol system. The experiment of 210 cm packed column with 150 cm diameter for the methanol/ethanol system [10] is equivalent to seven stages of the trayed column found from the rigorous simulation. The small number of trays does not give the composition gap between vapor and liquid phases in the middle of the column unless the volatility difference of light and heavy components is large like the methanol/*n*-propanol system.

CONCLUSION

We have proposed a new simulation procedure for the packed distillation, and examined its performance by comparison with the experimental results. The rate-based model composed of the differential equation of material balance and the rate equation of mass transfer for both liquid and vapor phases is utilized, because the packed column has continuous internal structure from top to bottom. Solving the differential equation is difficult due to the unknown boundary condition of the counter flow of vapor and liquid streams. The packed-column model of the differential equations is sequentially solved using an iterative computation. The computed results of the proposed model were compared with the experimental results for the systems of methanol/ethanol, ethanol/*n*-propanol and methanol/*n*-propanol, and the proposed procedure gives satisfactory prediction of the vapor and liquid compositions in the packed distillation column.

ACKNOWLEDGEMENTS

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NOMENCLATURE

A : column cross-sectional area [m^2]
a : volumetric interfacial area [m^{-1}]
c : concentration [mol m^{-3}]
G : vapor flow rate [mol s^{-1}]
J : mass flux [mol m^{-1} s^{-1}]
K : equilibrium constant [-]
k : mass transfer coefficient [m s^{-1}]
x : liquid composition of light component [mol fraction]
y : vapor composition of light component [mol fraction]
z : column length [m]

Greek Letter

α : relative volatility

Superscript

G : vapor phase
L : liquid phase

Subscript

e : equilibrium
G : vapor phase
j : column height
L : liquid phase
t : total

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