

Separation performance investigation of packed distillation columns using simple NEQ approach based on packing multicomponent efficiencies and effective mass transfer coefficients

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Abstract—A simple non-equilibrium modeling approach is proposed to simulate multicomponent distillation process in packed columns. The real behavior of the column is simply considered by the evaluation of interphase mass transfer rate based on the overall mass transfer coefficient. Two distinct methods are used to calculate this overall coefficient including the effective mass transfer coefficient method and the packing efficiency method. The modelling procedure consists of an iterative segment-wise algorithm implemented in a MATLAB home-code. For verification, the obtained composition profiles from a structured and a random packed column are compared with reported experimental data. Comparisons show that the packing efficiency-based model could acceptably predict the experimental profiles with an average relative deviation of 18% and 25% for structured and random packed columns, respectively. This confirms that our simple non-equilibrium approach is a reliable and robust model for the performance evaluation of packed columns.

Keywords: Packed Distillation Column, Multicomponent Separation, Simple Non-equilibrium Modeling, Overall Mass Transfer Coefficient, Packing Efficiency

INTRODUCTION

Among various separation techniques, distillation is the most widely used industrial method for separation goals [1]. Distillation columns are extensively applied in chemical, petrochemical, petroleum, and natural gas industries [2]. According to internal devices which are applied as phase contactors, distillation columns are categorized as random or structured packed columns and trayed or plate columns. The vapor and the liquid are in continuous contact in the packed columns, while stepwise contact between phases occurs in plate towers [3]. To achieve the efficient mass transfer between phases, trayed towers are designed to provide enough liquid holdup. In contemporary industrial uses, packed columns are applied more than trayed towers, especially when low-pressure drops across the column are required. In packed towers, a large surface area per unit volume is provided to facilitate the liquid-vapor mass transfer. Recently, packed distillation columns with structured packings have gained more attention for development of the existing trayed columns [4]. Structured packings are a good substitute for existing trays when more capacity or higher degree of separation is required [5].

The initial investment related to installed capacity and operational costs due to energy usage of distillation operation are significant [6]. Therefore, distillation columns should be designed precisely as possible to achieve the optimum operational conditions. Since conducting experiments to determine design parameters or evalu-

ate an existing design is very expensive and time-consuming, designers have often used the simulation tool to examine their idea for the process advancement. In fact, simulation is a robust tool for the process analysis and the equipment initial design. A trustworthy model is essential for the performance evaluation of the distillation process [7].

The modeling of distillation is not new. Depending on the assumptions, distillation modeling approaches vary from the simple to the quite complex. Until now, many of the challenging problems related to the distillation process modeling have been widely investigated. The equilibrium (EQ) stage model is the most common method for the simple simulation of the distillation process [3]. For more than a century, distillation columns have been simulated by the EQ stage concept [8]. In this approach, it is assumed that both of the vapor and the liquid phases are perfectly mixed so that the outlet streams from a theoretical (ideal) stage reach the equilibrium state. Since a detailed equipment design is not required, this model is a simple on-hand modeling approach. Indeed, a minimum amount of data (only data for the calculation of K-values and enthalpies) are required for the EQ modeling of the distillation process. Mass, equilibrium, summation and heat (MESH) relations make the governing equations of the EQ stage model [9]. The EQ modeling approach is considered as a conventional method to simulate packed distillation columns with introducing HETP (the height equivalent to a theoretical plate) concept as a something similar concept to the stage efficiency in trayed columns [10]. According to this, the packed tower is modeled similar to a staged column, so that the packed height is divided into a number of sections, each of them considered as a discrete stage. Although the HETP concept is widely applied, no theoretical justifi-

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cation is available and this leads to the deviation from experimental data [11]. In fact, the performance of the EQ modeling approach in the simulation of packed columns is extremely dependent to the precision of HETP values.

Although the EQ model has been applied as a conventional approach for steady-state simulation of the distillation process, several shortcomings are observed due to applied assumptions. In fact, actual stages significantly deviate from ideal stages, and outlet streams from a real tray or a packed section are rarely in equilibrium. Therefore, researchers have considered the non-ideality of real distillation columns in the modeling approaches. As previous studies have clearly shown, the actual separation in a distillation column depends on interphase mass transfer rates [12]. These rates correspond to the measure of the deviation of vapor and liquid streams from the equilibrium state. In packed distillation towers, the performance of mass transfer is often expressed by HETP values. However, the HETP concept is not directly applicable in multicomponent distillations, because the mass transfer rates are different for various species in multicomponent mixtures. A proper alternative for HETP is HTU (height of a transfer unit) concept [13]. This concept represents the mass transfer efficiency of the packed bed. HTU can be correlated much more easily than HETP and successfully used in the design of packed columns for separating binary mixtures. However, it has been experimentally shown that HTU values are commonly different for each component in multicomponent mixtures [14]. It means that each component has diverse mass transfer efficiency along the packed bed. To overcome this problem in a multicomponent packed distillation process, two main approaches are commonly suggested: the efficiency-based modified EQ method, and the non-equilibrium (NEQ) stage method, known as the rate-based model. As a first suggestion, the multicomponent efficiency calculations [15] are introduced into the EQ modeling approach. Accordingly, the separation efficiency of each component is predicted in any calculation segment. The efficiency-based modified EQ model is one of the conventional approaches to consider the mass transfer phenomena in the distillation process [8]. The characteristic feature of this approach is that the multicomponent efficiencies are calculated together with the whole modeling procedure. In the second suggestion, the rate based approach [16-18] is used in which the actual mass transfer rates are directly determined for a given packing section or a real plate. However, the rate-based model is quite heavy to solve. Meanwhile, many physical properties, such as diffusion coefficients, surface tension, thermal conductivities, and viscosities, are required in this approach. Indeed, the rate-based modeling approach gives more detailed results about column separation at the expense of heavier computational cost and more equipment design details than EQ stage approach.

In recent years, different researchers have been motivated to apply efficiency calculations along with EQ modeling approaches to consider the non-ideal nature of multicomponent distillation process. The applying of multicomponent plate efficiencies on the platform of EQ stage model was initially introduced by Aittamaa [19]. This modeling approach was later developed further by Ilme [20]. The efficiency-based methods have been widely studied by Klemola [21], Jakobsson [22], and also applied for industrial col-

umns by Ilme et al. [23], Jakobsson et al. [24]. Although several works are dedicated to multicomponent efficiency calculations, most of them have focused on the modeling of plate columns, and the packed distillation columns are seldom modeled using this approach. Keskinen et al. [25] used an EQ model with multicomponent efficiency factors for the evaluation of the separation performance of packed distillation columns; however, they believed that their method still needed extra work to be verified with more experimental data.

In our previous study [26], we presented a simple NEQ model based on rigorous efficiency calculations for the simulation of plate distillation columns. In this model, the phase equilibrium relations in the EQ stage method are replaced with the interphase mass transfer equations based on overall mass transfer coefficients. The overall mass transfer coefficient is simply calculated from the simultaneous solution of the vapor phase material balance and the Murphree efficiency definition. The main characteristic of the presented model is to combine advantages of the efficiency-based modified EQ model and the rate-based NEQ model to obtain an effective and appropriate approach for the modeling of the distillation process. In the proposed model, the behavior of real plates is initially estimated in the form of stage efficiencies, and then column separation performance is obtained. In the present work, we use this efficiency-based NEQ approach for the modeling of packed distillation columns. According to this, the mass transfer in any packed segment is considered by multicomponent efficiency calculations to correct the deviation from the equilibrium stage assumption. Besides, another simple NEQ model based on effective mass transfer coefficients is also applied for the further evaluation of the proposed efficiency-based NEQ model. In this approach, the effective mass transfer coefficients are initially calculated for each phase, and next they are combined to compute the overall mass transfer coefficient. So, it can be said that the common face of both implemented NEQ methods is that their modeling procedure is based on the evaluation of interphase mass transfer rates according to the overall mass transfer coefficients. The key feature of these modeling approaches is that the non-equilibrium nature of the distillation process is considered while the structure of EQ stage method is maintained.

Therefore, our aim is the rigorous simulation of packed distillation columns by using two simple NEQ approaches based on the simple calculation of interphase mass transfer rates. In this paper, a detailed comparison between results of our NEQ models and reported measured data is performed for two different packed distillation columns: a structured packed column as case study I and a random packed column as case study II. By using these methods, the mentioned packed columns are modeled in the same way as a staged column so that the packed height is divided into a number of sections, each of which may be modeled as a discrete NEQ stage. In this way, the separation performance of both columns is obtained, and then the estimated separations are compared with actual measurements along the packed beds. Accordingly, the column design can be analyzed, and could be modified if needed.

MODEL DESCRIPTION

Basically, two classes of approaches are suggested for the packed

column modeling: the discrete approach and the continuous approach [27]. In the discrete method, the packed bed is divided into several sections so that each section is treated as a stage in the plate column, and the model contains a set of nonlinear algebraic equations as governing equations. Therefore, the stage-wise modeling approaches are applicable in the simulation of continuous contact devices as well as staged contactors. However, in the continuous method, the packed column is considered as a continuous contactor while the differential balance equations are written for any small element of packing. So, the model consists of a set of differential equations that are solved using a numerical integration scheme.

In the current work, we apply the discrete approach. Accordingly, the packed column is modeled in the same way as a staged column where the packed height is vertically divided into a number of control volumes, each of them can be considered as a discrete stage. All of control volumes contain the liquid and the vapor phase with homogeneous temperature and composition, and are referred to as packing segments. In this way, the balance equations for each packing segment are similar to corresponding equations for a single stage in a plate column. In the simulation procedure, the mass transfer stages can be identified with these packing segments. The segments are interrelated via mass and energy balance equations. The configuration of each segment is represented in Fig. 1.

In this work, the non-equilibrium behavior of a packed distillation column is described by using the interphase mass transfer rates calculated based on the vapor phase overall mass transfer coefficient. So, the packed column consists of a sequence of non-equilibrium stages, each of which represents a section of packing. Indeed, the overall mass transfer coefficient approach is a simplified rate-based approach in which the temperature of the liquid and the vapor phase is assumed to be the same. In addition, the temperature and composition at the interface are not variable in this approach.

The key feature of this simple NEQ model is that the structure of the EQ stage model is preserved while the non-ideality of the distillation process due to mass transfer effects is considered. According to this approach, the material balance equations for each segment are split into two parts, one for each phase, and solved

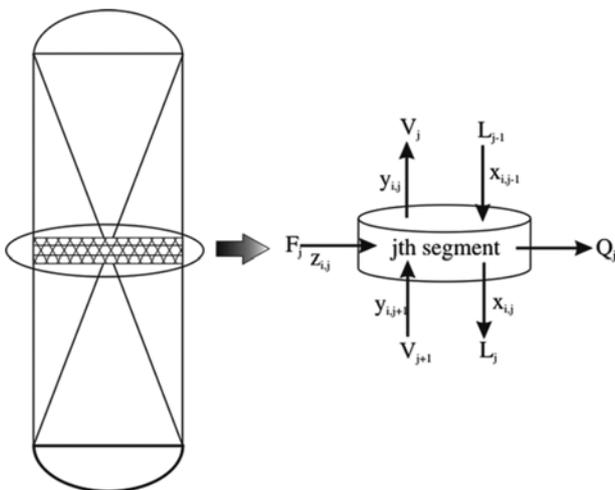


Fig. 1. Schematic representation of a segment in the packed bed.

simultaneously with energy balance equation. Several assumptions have been used to simplify the model, including:

- 1) Both phases are perfectly mixed in each segment,
- 2) Vapor-liquid equilibrium is established only at the interface,
- 3) The mass transfer resistance mainly exists in the vapor phase,
- 4) The finite flux effects on the mass transfer coefficients are ignored, then the low flux mass transfer coefficients are applied into equations of the model,
- 5) The interphase heat transfer rates are assumed to be negligible,
- 6) The condenser and the reboiler are treated as equilibrium stages.

1. Governing Equations of the Simple NEQ Model

To consider the non-equilibrium behavior of a real packed bed, it is necessary to include the interface mass transfer effects in the component material balances written for any packing segment. Mass transfer on a two-phase contact segment may be described by two distinct material balance equations, one written for the liquid phase and one for the vapor phase. The component balance equations for each phase are stated as:

$$l_{i,j-1} - l_{i,j}(1+r_j^L) + f_{i,j}^L - N_{i,j}^L a_j = 0 \quad (1)$$

$$v_{i,j+1} - v_{i,j}(1+r_j^V) + f_{i,j}^V + N_{i,j}^V a_j = 0 \quad (2)$$

where $l_{i,j}$, $v_{i,j}$ and $f_{i,j}$ are component flow rates for liquid, vapor and feed, respectively, and r_j is the dimensionless sidestream flow rate. The term related to feed ($f_{i,j}$) should be considered in both equations since feed may enter either phase. Writing a material balance around the entire interface resulted in Eq. (3):

$$N_{i,j}^L = N_{i,j}^V = N_{ij} \quad (3)$$

where N_{ij} is the interphase molar flux that is determined by following simple expression in place of equations for rigorous multi-component mass transfer rate used in rate-based approach:

$$N_{i,j} = c^V K_{ij}^{OV} (y_{ij}^* - y_{ij}) \quad (4)$$

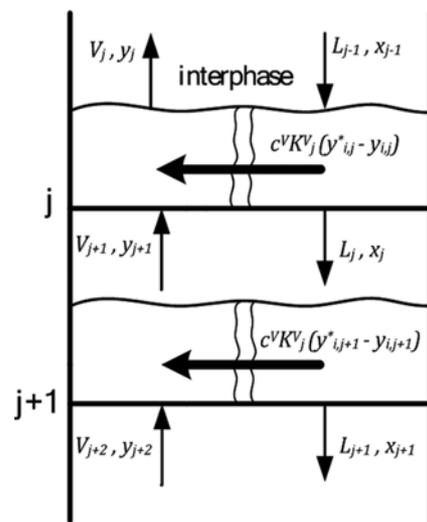


Fig. 2. Schematic representation of the interphase mass transfer in a simple NEQ multistage operation.

In the above equation, $y_{i,j}^* = K_{i,j} x_{i,j}$ where $K_{i,j}$ is the K-value of component i at stage j , and K_{ij}^{OV} is the overall mass transfer coefficient for the vapor phase. Eq. (4) is obtained based on the relation between the mass transfer driving force and the equilibrium condition. According to this relation, the rate of mass transfer decreases while conditions proceed toward equilibrium. Fig. 2 schematically depicts the flow pattern inside the segments according to the inter-phase mass transfer effects [26].

The heat transfer rates in all segments are ignored, so the energy balance equations for our NEQ model are written similar to EQ model as follows:

$$H_j^V(1+r_j^V)\sum_{k=1}^c v_{k,j} + H_j^L(1+r_j^L)\sum_{k=1}^c l_{k,j} - H_{j+1}^V\sum_{k=1}^c v_{k,j+1} - H_{j-1}^L\sum_{k=1}^c l_{k,j-1} - H_j^F\sum_{k=1}^c f_{k,j} + Q_j = 0 \tag{5}$$

where c indicates the number of components of the mixture, and j represents the corresponding stage number. In the simulation, stage 1 corresponds to the condenser and stage N represents the reboiler. These end stages are considered as ideal stages even though equilibrium is not achieved along the packed bed. Therefore, the equations for these stages differ from other equations representing a general non-equilibrium stage. The equations for the condenser and the reboiler are presented in Table 1.

We used two different approaches to predict the overall mass transfer coefficients in Eq. (4): the method of effective mass transfer coefficients and the method of packing multicomponent efficiencies.

2. Method of Effective Mass Transfer Coefficients

According to this method, the “effective” mass transfer coefficients for the vapor phase and the liquid phase are combined to calculate the overall mass transfer coefficient for the vapor phase (K_{ij}^{OV}) as follows [28]:

$$\frac{1}{c^V K_{ij}^{OV}} = \frac{1}{c^V \kappa_{ij}^V} + \frac{K_{ij}}{c^L \kappa_{ij}^L} \tag{6}$$

where κ_{ij}^V and κ_{ij}^L are the effective mass transfer coefficients for the vapor and the liquid phase, respectively. These coefficients are obtained by the following equations:

$$\kappa_{ij}^V = \frac{1 - y_{ij}}{\sum_{p=1}^c (y_{pj} / k_{ip}^V)} \tag{7}$$

$$\kappa_{ij}^L = \frac{1 - x_{ij}}{\sum_{p=1}^c (x_{pj} / k_{ip}^L)} \tag{8}$$

In these equations, k_{ij} represents the binary mass transfer coefficients that are estimated by using correlations correspond to the type of packings applied in the column.

3. Method of Packing Multicomponent Efficiencies

In this approach, the overall mass transfer coefficient for the vapor phase is determined using a specific relation obtained from the simultaneous solution of the vapor phase material balance and the definition of Murphree efficiency as follows [29]:

$$\frac{c^V K_{ij}^{OV}}{V_j} = \frac{E_{ij}^{MV}}{1 - E_{ij}^{MV}} \tag{9}$$

where E_{ij}^{MV} represents the Murphree efficiency of component i at segment j . As mentioned, efficiencies are not the same for all components on each segment in multicomponent mixtures. So, the estimation of K_{ij}^{OV} by Eq. (9) needs multicomponent efficiency calculations. For a multicomponent dilute system in a packed distillation column, the vapor phase material balance equation is written as below in the form of matrix notation:

$$V \frac{d(y)}{dh} = -(J^V) a_e A_c \tag{10}$$

where a_e is the effective interfacial area of the packing, and A_c is the column surface area. By substituting the diffusion flux vector, (J^V) , with the matrix of overall mass transfer coefficients, $[K^{OV}]$, the following equation is obtained:

$$V \frac{d(y)}{dh} = c^V [K^{OV}] (y^* - y) a_e A_c \tag{11}$$

This equation can be expressed as Eq. (12) by introducing the concept of overall heights of transfer units (HTUs):

$$V \frac{d(y)}{dh} = [H^{OV}]^{-1} (y^* - y) \tag{12}$$

where y^* represents the equilibrium vapor composition. Because y^* is different for each packing segment, Eq. (12) should be numerically integrated to obtain the vapor composition profile along the packed height. To avoid numerical integration, the term $(y^* - y)$ is approximated with the arithmetic mean value for a limited seg-

Table 1. Equations for the condenser and the reboiler as ideal stages

	Condenser (j=1)	Reboiler (j=N)
Material balance	$l_{i,1} + v_{i,1} - v_{i,2} - f_{i,1} = 0$	$l_{i,N} + v_{i,N} - l_{i,N-1} - f_{i,N} = 0$
Energy balance	$\sum_{k=1}^c l_{k,1} - RR \sum_{k=1}^c v_{k,1} = 0$	$\sum_{k=1}^c l_{k,N} - W = 0$
Partial	$K_{i,1} \frac{l_{i,1}}{\sum_{k=1}^c l_{k,1}} - \frac{v_{i,1}}{\sum_{k=1}^c v_{k,1}} = 0$	
Equilibrium	$\sum_{p=1}^c \left(K_{p,1} \frac{l_{p,1}}{\sum_{k=1}^c l_{k,1}} \right) - 1 = 0$ (bubble point equation)	$K_{i,N} \frac{l_{i,N}}{\sum_{k=1}^c l_{k,N}} - \frac{v_{i,N}}{\sum_{k=1}^c v_{k,N}} = 0$
Total	$\frac{l_{i,1}}{\sum_{k=1}^c l_{k,1}} - \frac{v_{i,1}}{\sum_{k=1}^c v_{k,1}} = 0$ (i=2: c)	

ment height [25]. This approximation leads to following equation for the segment number j :

$$(y)_j - (y)_{j+1} = h_j [H^{OV}]_j^{-1} \left(\frac{[K]_j(x)_j + [K]_{j-1}(x)_{j-1}}{2} - \frac{(y)_j + (y)_{j+1}}{2} \right) \quad (13)$$

where $(y)_j$ and $(x)_j$ denote the concentration vector of the vapor and the liquid leaving the segment j , and $(y)_{j+1}$ and $(x)_{j-1}$ represent the concentration vector of the vapor and the liquid entering the segment j . $[K]_j$ and $[K]_{j-1}$ are the diagonal matrix of K -values corresponding to liquid concentrations x_j and x_{j-1} , respectively. $[H^{OV}]$ corresponds to the matrix of overall HTUs in the segment j and h_j is the height of segment j . Now the packing efficiency may be defined similarly to the Murphree vapor phase plate efficiency as follows [30,31]:

$$E_j^{MV} = \frac{y_j - y_{j+1}}{y_j^* - y_{j+1}} \quad (14)$$

Finally, the following expression is obtained to predict packing multicomponent efficiencies based on Eqs. (13), (14) for the segment j :

$$(E^{MV})_j = [A]_j \frac{h_j}{2} [H^{OV}]_j^{-1} \{ [K]_j(x)_j + [K]_{j-1}(x)_{j-1} - (y)_j - (y)_{j+1} \} \quad (15)$$

where $[A]_j$ is a diagonal matrix as follow, and its elements are the reciprocals of term $(y_j^* - y_{j+1})$ for $c-1$ components:

$$[A]_j = \begin{bmatrix} \frac{1}{y_{1,j}^* - y_{1,j+1}} & 0 & \dots & 0 \\ 0 & \frac{1}{y_{2,j}^* - y_{2,j+1}} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \frac{1}{y_{c-1,j}^* - y_{c-1,j+1}} \end{bmatrix} \quad (16)$$

Eq. (15) is the basic equation for the efficiency-based NEQ modeling of a packed distillation column. The main term in this equation is the overall HTU matrix, $[H^{OV}]$, that should be calculated before the estimation of segment efficiencies. $[H^{OV}]$ can be calculated based on multicomponent mass transfer models which are best described with Maxwell-Stefan diffusion equations in connection with the two-film theory as follow:

$$[H^{OV}] = [H^V] + A[H^L], \quad A = [K] \quad (V/L) \quad (17)$$

where $[H^V]$ and $[H^L]$ are the HTU matrix for the vapor and the liquid phases, respectively. They are defined as:

$$[H^V] = \frac{[R^V]u_{sV}}{a_e} \quad (18)$$

$$[H^L] = \frac{[R^L]u_{sL}}{a_e} \quad (19)$$

where u_{sV} and u_{sL} are the superficial velocity for the vapor and the liquid phases, respectively. $[R]$ is the inverse matrix of mass transfer coefficients that its elements are given by:

$$R_{ii} = \frac{z_i}{k_{ic}} + \sum_{\substack{p=1 \\ k \neq i}}^c \frac{z_p}{k_{ip}} \quad (20)$$

$$R_{ij} = -z_i \left(\frac{1}{k_{ij}} + \frac{1}{k_{ic}} \right)$$

In this equation, z is the mol fraction of the appropriate phase and k_j is the binary mass transfer coefficient of the same phase.

After the evaluation of the overall HTU matrix, the HETP values could be determined by following relation [15]:

$$\text{HETP} = H \left(\frac{\ln A}{A-1} \right) \quad (21)$$

4. Binary Mass Transfer Coefficients and the Interfacial Area

It is clear that both methods for the calculation of overall mass transfer coefficients require the estimation of binary mass transfer coefficients. Several correlations have been proposed for the calculation of mass transfer coefficients and the interfacial area in packed distillation columns. According to packing types, we applied two different correlations for the prediction of mass transfer coefficients: correlation of Bravo et al. [32] for structured packings, and correlation of Onda et al. [33] for random packings.

Correlation of Bravo et al. [32] for Structured Packings:

According to this correlation, binary mass transfer coefficients for each phase are estimated as follows:

$$k^V = Sh_V D^V / d_{eq} \quad (22)$$

$$k^L = 2 \sqrt{D^L u_{Le}} / (\pi S) \quad (23)$$

where Sh_V is the Sherwood number, d_{eq} is the equivalent diameter of a channel, S is the packing corrugation spacing (channel side), u_{Le} is the effective liquid velocity, and D is the diffusion coefficient. The dimensionless groups used in above equations are defined as:

$$\begin{aligned} Sh_V &= 0.0338 Re_V^{0.8} Sc_V^{0.333} \\ Re_V &= d_{eq} \rho^V [(u_{Ve} + u_{Le}) / \mu^V] \\ Sc_V &= \mu^V / (\rho^V D^V) \end{aligned} \quad (24)$$

The method of Bravo et al. [32] assumes that the surface is completely wetted. Therefore, the interfacial area per unit of packing volume is equal to the specific packing surface ($a_e = a_p$).

Correlation of Onda et al. [33] for Random Packings: The Onda correlation predicts the mass transfer coefficients by the following equations:

$$\frac{k^V}{a_p D^V} = A \frac{Re_V^{0.7} Sc_V^{0.333}}{(a_p d_p)^2} \quad (25)$$

$$k^L \left(\frac{\rho^L}{\mu^L g} \right)^{0.333} = 0.0051 \frac{(Re_L')^{0.667}}{\sqrt{Sc_L}} (a_p d_p)^{0.4} \quad (26)$$

where d_p is the nominal packing size, and a_p is the specific surface area of the packing. The parameter A is a constant that takes the numerical value 2.0 if the nominal packing size is less than 0.012 m and has the value 5.23 if the nominal packing size is greater than (or equal to) 0.012 m. The dimensionless groups used to above relations are defined as:

$$Re_V = \frac{\rho^V u_V}{\mu^V a_p}, \quad Re_L' = \frac{\rho^L u_L}{\mu^L a_e} \quad (27)$$

$$Sc_V = \frac{\mu^V}{\rho^V D^V}, \quad Sc_L = \frac{\mu^L}{\rho^L D^L}$$

The parameter a_v is the interfacial area density (m^2/m^3 packing) that is determined as follows:

$$a_v = a_p \left(1 - \exp \left\{ -1.45 \left(\frac{\sigma_c}{\sigma} \right)^{0.75} \frac{Re_L^{0.1} We_L^{0.2}}{Fr_L^{0.005}} \right\} \right) \quad (28)$$

where σ is the surface tension of the liquid and σ_c is the critical surface tension of the packing. The dimensionless groups are calculated as follows:

$$Re_L = \frac{\rho^L u_L}{\mu^L a_p}, \quad Fr_L = \frac{a_p u_L^2}{g}, \quad We_L = \frac{\rho^L u_L^2}{a_p \sigma} \quad (29)$$

The interfacial area (a_j) is given as the product of a_v in the volume

of the segment j as follows:

$$a_j = a_v v_j \quad (30)$$

where v_j is the volume of a packed segment represented by a NEQ stage.

SIMULATION PROCEDURE

The simulation procedure of a packed distillation column starts with dividing the packed height into a number of segments. The segments are considered then as a sequence of mass transfer stages in the calculations. Simulations consist of several steps that are repeated for all packing segments. In each step, a set of values for the overall mass transfer coefficients is initially obtained from either

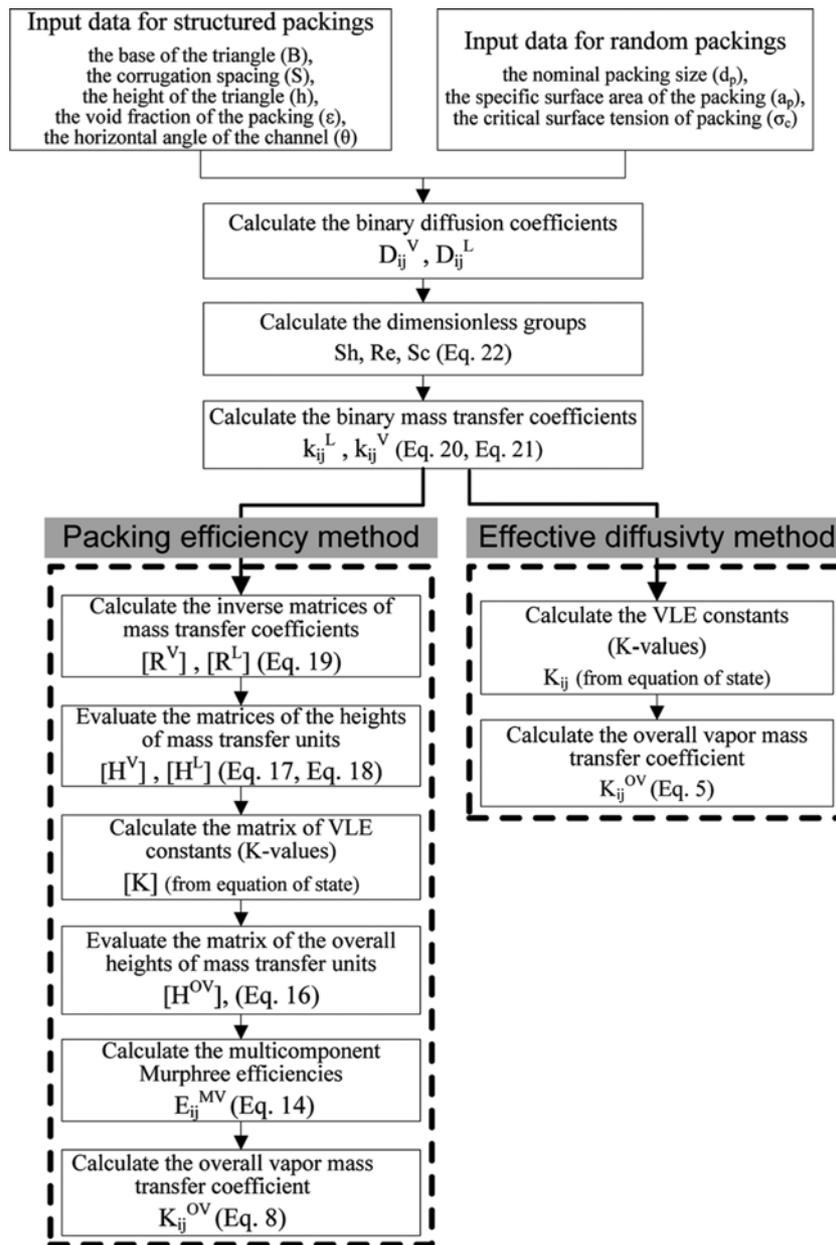


Fig. 3. The segment-wise calculation procedure for calculating the overall mass transfer coefficients.

effective mass transfer coefficients or packing multicomponent efficiencies. Fig. 3 represents step by step procedures for the calculation of the segment-wise overall mass transfer coefficients using both proposed methods.

The obtained overall mass transfer coefficients are used to estimate the rate of mass transfer for any calculation segment. The calculated mass transfer rates are then introduced to the mass balance equations to correct the equilibrium assumption. Eventually, whole equations of the model are iteratively solved to obtain the profiles of compositions and temperature along the packed height. The sequence of simulation steps related to each NEQ model is depicted in Fig. 4 as flowcharts.

As it can be seen in Fig. 4(a), two calculation loops are encoun-

tered in the efficiency-based NEQ model. In the outer loop, overall mass transfer coefficients are determined using each set of estimated efficiencies. Then, by using these values, whole model equations are solved in the inner loop to achieve the converged values of compositions and temperatures. Next, the new efficiencies are calculated again in the outer loop, and this procedure is repeated until the mathematical model of the whole packed column is converged. On the other hand, the NEQ model based on effective mass transfer coefficients only includes an individual calculation loop, so that calculations proceed with determined overall mass transfer coefficients in each iteration to reach the final results (see Fig. 4(b)). The modified Newton-Raphson method [34] has been used to simultaneously solve the set of equations obtained

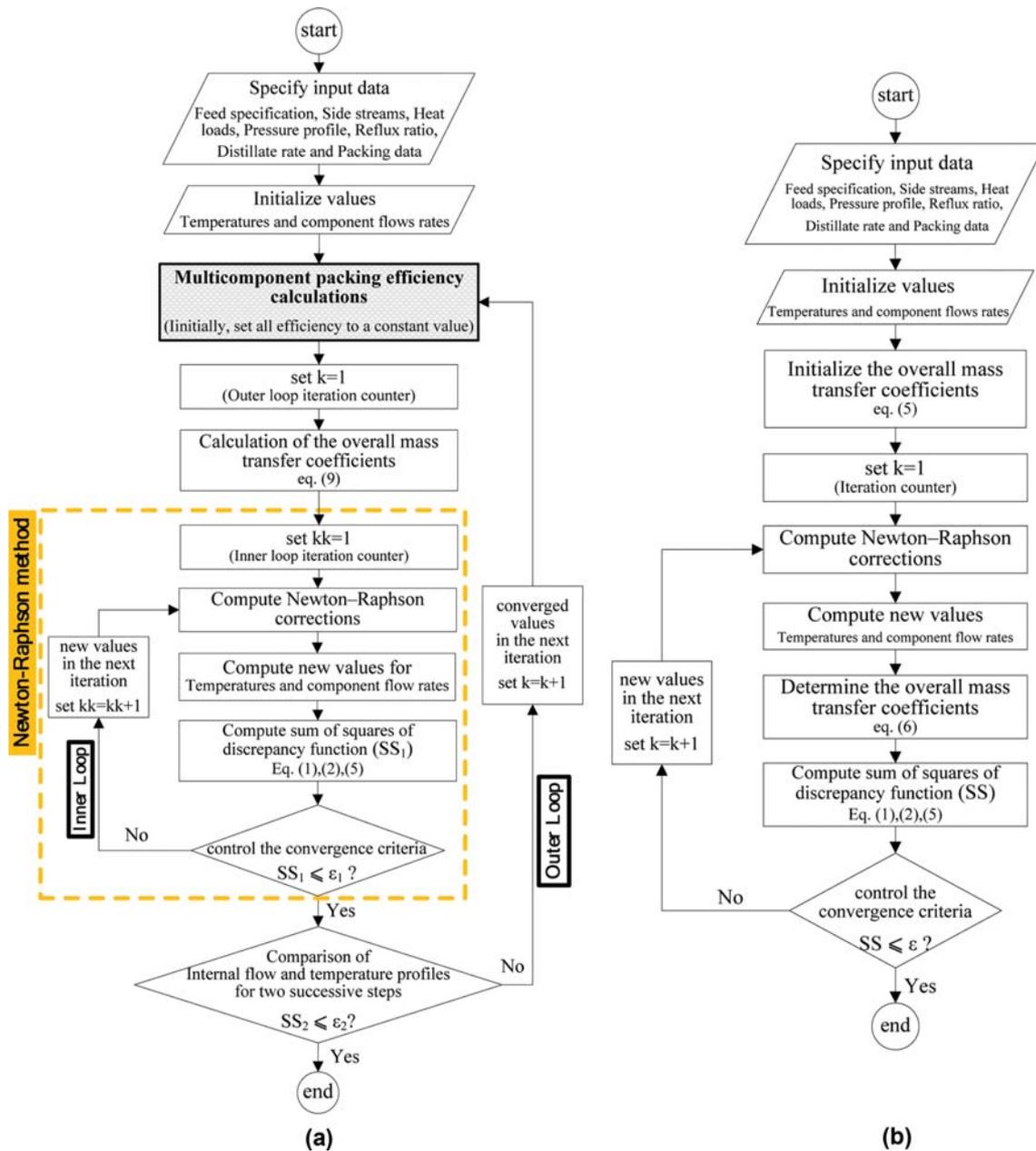


Fig. 4. The sequence of simulation steps. (a) The multicomponent efficiency-based NEQ model. (b) The NEQ model based on effective mass transfer coefficients.

for each NEQ model. The simulation process based on both NEQ approaches has been implemented in our developed home-code within MATLAB environment. By applying this computational code, it is possible to simulate a packed column with any number of segments, various packing types and sizes, and column diameter etc. Furthermore, the model is known exactly by using this home-code, so that it can be modified to examine the validity of various assumptions. There is also more flexibility when convergence problems are encountered.

METHOD OF VALIDATION

We used two experimental packed distillation columns to evaluate our modeling approaches and validate simulation results. The first case (presented by Mori et al. [35]) is a structured packed column that separates a non-ideal ternary mixture containing methanol, ethanol, and water. A schematic representation of mentioned packed distillation column. As shown, the feed is introduced at the middle of the column; therefore, the length of enrich-

ing and stripping sections is equal. Each of these sections contains six structure packing elements. The geometry of applied packings is similar to other commercial corrugated sheet-type packings, but sheets are sandwiched by gauze. Thus, the wetting characteristics of applied packings are close to that of gauze-type packings. The second column (introduced by Arwikar [36]) separates another non-ideal mixture consisting of acetone, methyl acetate, and methanol in a random packed bed containing Raschig ring packings. The column operates under total reflux condition in the normal atmospheric pressure. The total reflux operation is stabilized so that the measured internal flow rates are equal to 0.019 mol/s. A simplified schematic of this laboratory-scale distillation column is shown in Fig. 5(b).

The specifications of both packed columns in addition to geometries of the packing elements are presented in Table 2(a), (b). The operating conditions and product compositions required for the simulation of continues distillation process in the case study I are given in Table 3(a).

As mentioned, the packed column in the case study II operates

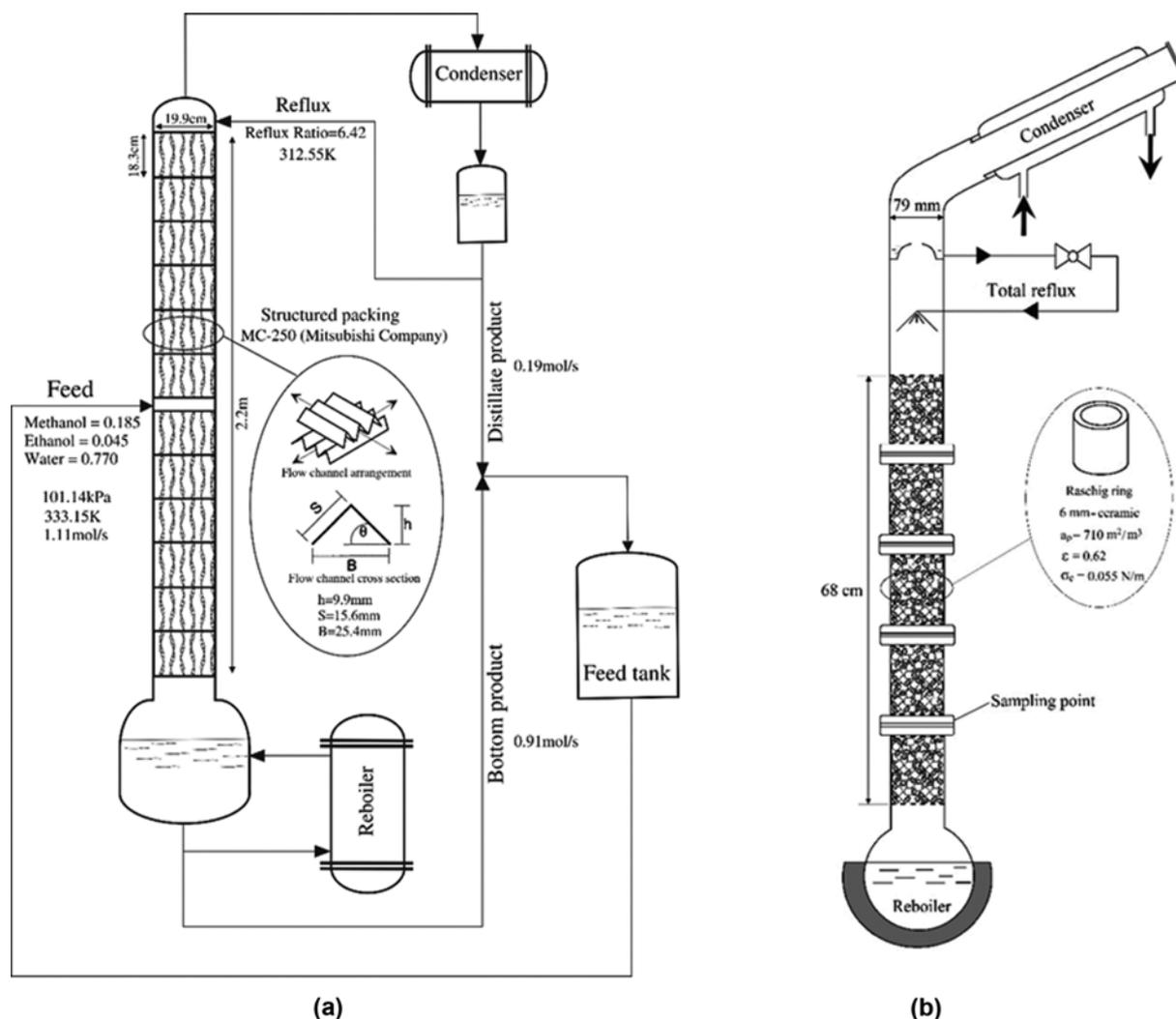


Fig. 5. Schematic representation of mentioned packed columns in addition to packing specifications. (a) Structured packed column-case study I (Methanol-Ethanol-Water system). (b) Random packed column-case study II (Acetone-Methyl Acetate-Methanol system).

Table 2. Specifications of mentioned packed columns in addition to information about packing elements

(a) Structured packed column (case study I)		(b) Random packed column (case study II)	
Column specification		Column specification	
Column height	3 m	Packed height	68 cm
Packed height	2.2 m	Diameter	79 mm
Diameter	21 cm	Packing elements	
Packing elements		Type	Random packing
Type	MC-250 (Mitsubishi Company)	Nominal packing size	Raschig ring
Element diameter	0.199 m	Specific surface area	0.25 in (6 mm)
Element height	0.183 m	Material	710 m ² /m ³
Height of triangle	9.9×10 ⁻³ m	Critical surface tension	Ceramic
Base of triangle	25.4×10 ⁻³ m	Void fraction	0.055 N/m
Corrugation spacing	15.6×10 ⁻³ m		0.62
Specific surface area	250 m ² /m ³		
Void fraction	0.98		
Channel flow angle	45°		

Table 3. Operating conditions of mentioned packed distillation columns

(a) Structured packed column: continuous operation			(b) Random packed column: pseudo-continuous operation		
Specification	Value		Specification	Value	
Feed flow rate	1.11 mol/s		Feed flow rate	1.9×10 ⁻⁴ mol/s	
Feed composition (mole fraction)	Methanol	0.185	Feed composition (mole fraction)	Acetone	0.165
	Ethanol	0.045		Methyl acetate	0.234
	Water	0.770		Methanol	0.600
Feed temperature	333.15 K		Feed temperature	Saturated temp.	
Feed entrance location	1.1 m (from top)		Feed entrance location	58 cm (from top)	
Feed quality	Liquid		Feed quality	Liquid	
Column pressure	101.4 kPa		Column pressure	101.4 kPa	
Distillate flow rate	0.19 mol/s		Distillate flow rate	F/2=9.5×10 ⁻⁵ mol/s	
Reflux ratio	6.42		Reflux ratio	200	
Reflux temperature	312.55 K		Reflux temperature	Saturated temp.	

in the total reflux condition. The simulation of total reflux operations is complicated by the fact that there is no feed to the column at steady state. To overcome this problem, pseudo-continuous approach is applied. According to this approach, the total reflux operation is simulated by common approaches for the simulation of continuous distillation processes so that an arbitrary value with negligible flow in comparison with internal flow rates is chosen as feed flow rate. The composition and entrance location of feed then correspond with conditions of one sample point for measuring compositions along the column. Indeed, the simulated composition profile of the total reflux run satisfies this specified composition. Since the column is operated at total reflux, the reflux flow rate determines the internal flow rates of vapor and liquid streams on each section. Therefore, the reflux ratio is determined so that the calculated internal flow rates are adjusted to the experimentally measured value (0.019 mol/s). The input parameters for pseudo-continuous simulation of random packed column in case study II are given in Table 3(b).

The physical properties of pure components and mixture are estimated by using various methods (see Table 4). Correlations for the estimation of binary mass transfer coefficients and the effective interfacial area correspond to applied structured packings are also presented in Table 4.

The simulation model of the column is specified by defining the thermodynamics of the system, the feed rate, the condition and composition of the feed, the column geometry and the packing specifications. Since both considered mixtures are very non-ideal, the gamma/phi approach [38] is used to describe the vapor-liquid phase equilibrium (VLE). According to this, the vapor phase fugacity coefficients are computed by the Soave modification of Redlich-Kwong (SRK) equation of state [39], while the liquid phase activity coefficients are calculated using two different models, including the UNIFAC group contribution method [40] and NRTL method [41]. In addition, the vapor pressure is determined by Antoine equation [42]. The NRTL parameters applied in our simulations are listed in Table 5. These parameters are used along with $G_{ij} =$

Table 4. Methods for estimating physical and mass transfer properties [37]

Physical properties	
Vapor molar density	Equation of State (SRK)
Liquid molar density	Modified Rackett method
Pure gas viscosity	Chung method
Mixture gas viscosity	Wilke method
Pure liquid viscosity	Correlation based on experimental data
Mixture gas viscosity	Grunberg and Nissan method
Pure surface tension	Sastri-Rao method
Mixture surface tension	Tamura method
Mass transfer properties	
Binary gas diffusion coefficient	Brokaw method
Binary liquid diffusion coefficient	Reddy and Doraiswamy method
	Bravo et al. [32] for structured packings
Binary mass transfer coefficient	Onda et al. [33] for random packings

Table 5. The NRTL parameters for binary mixtures at 101.3 kPa

Case study I; Methanol-Ethanol-Water [43] ($\tau_{ij}=B_{ij}/T$)						
Component i	Component j	B_{ij} [K]		B_{ji} [K]		α_{ij}
Water	Ethanol	624.92		-29.17		0.294
Water	Methanol	594.63		-182.61		0.297
Ethanol	Methanol	73.41		-79.17		0.303
Case study II; Acetone-Methyl acetate-Methanol [44] ($\tau_{ij}=a_{ij}+b_{ij}/T$)						
Component i	Component j	a_{ij}	a_{ji}	b_{ij} [K]	b_{ji} [K]	α_{ij}
Acetone	Methanol	0	0	101.886	114.135	0.3
Acetone	Methyl acetate	1.4101	-1.9348	-592.968	835.809	0.3
Methanol	Methyl acetate	0	0	130.505	234.866	0.3

$\exp(-\alpha_{ij}\tau_{ij})$.

RESULTS AND DISCUSSION

According to our simple NEQ model, two experimental packed distillation columns conducted by Mori et al. [35] and Arwihar [25,36] are used to implement the simulation procedures. The main purpose of simulations is to evaluate the separation performance of considered packed columns under various conditions by the efficiency-based NEQ model and the effective mass transfer NEQ model. In the first step, the effect of packed segment size and liquid activity model are investigated on the prediction of the separation performance of the structured packed column (case study I). Since the efficiency-based NEQ model involves two calculation loops and several matrix calculation operations, the complete simulation of the packed column with this model requires more computation time compared to the simulation by the effective mass transfer model. However, the simulation with the efficiency-based approach gives more detailed results about the column separation performance, such as packing efficiency and HTUs. It also gives more precise information about the mass-transfer phenomena such as the degree of backmixing on each segment. Therefore, the proper segment size and the appropriate activity model are cho-

sen based on the effective mass transfer approach. According to these results, two NEQ models are compared, eventually. For more investigation of our proposed NEQ models, the results of HETP-based EQ modeling approach are also presented.

1. The Segment Size

The number of segments can be considered as a parameter that considers the backmixing in packed distillation columns. When the number of segments is very high, basically no backmixing occurs in the column, and, therefore, the separation becomes maximum. Since backmixing and other non-ideal phenomena do exist in real columns, an appropriate number of segments should be used. Indeed, the accuracy of the method is related to the number of calculation segments specified for a certain packing height. Therefore, the selection of this factor could have a significant impact on simulation results. Consequently, it is one of the parameters that should be cautiously chosen in the mass transfer models. However, this factor cannot be determined in advance. When experimental data are available, the simulation results should be compared to these data to determine the optimal number of segments. Accordingly, the simulations are performed several times while a different number of segments are used in each run. Therefore, the size of segments is decreased step by step to minimize the differences between simulation and observed data. The resulting profiles of tem-

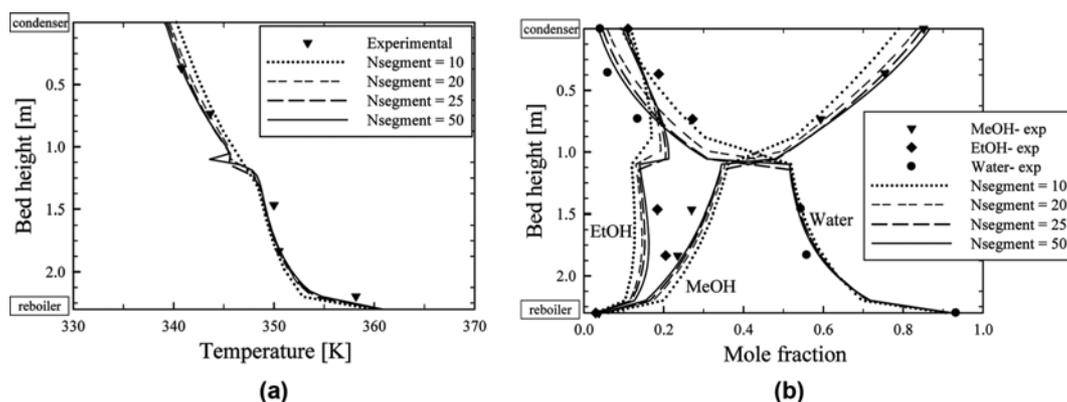


Fig. 6. The resulting profiles from the effective mass transfer NEQ model for several segment sizes in addition to some experimental data. (a) Temperature profiles. (b) Liquid composition profiles.

perature and component compositions in addition to experimental data along the column are presented in Fig. 6(a), (b). Simulations are performed based on the effective mass transfer NEQ model.

As shown in Fig. 6, there is a significant difference in the temperature and composition profiles between the model results and the experimental data, especially for large segment sizes. However, this difference at the top and the bottom of the column is less than that in the middle section. It can be obviously seen that the profiles obtained by the model incline to experimental results, as the size of calculation segments decreases. Since the size of segments directly affects the total computation time required for the convergence, excessive increase in the number of segments is also not desirable. According to the obtained profiles for different segment sizes, when the total packed height is divided into 25 segments (meaning 8.8 cm for each segment), experimental profiles are predicted properly. Therefore, this number of segments is used for further simulations.

2. The Liquid Activity Model

The thermodynamic equilibrium constant (K -value) is normally obtained from a variety of methods depending on the system complexity. For most gas processing applications, an equation of state is often used, and this directly yields the fugacity coefficients. When the liquid phase becomes more non-ideal, some applications will require a Gibbs excess free energy model, which gives the fugacity coefficients through the activity coefficients. Therefore, it is necessary to select appropriate methods for estimating thermodynamic

properties of the system. In non-ideal systems, interactions exist between components that differ from other components in respect to size, character, polarity and hydrogen bonding. The vapor-liquid equilibrium (VLE) of these mixtures is much more complicated than systems including non-polar species without hydrogen bonding such as hydrocarbons. Indeed, in a thermodynamically non-ideal system, the thermodynamic and physical properties of the vapor and the liquid phases are quite different for each component.

The considered structured packed column in case study I separates a ternary mixture consisting of methanol, ethanol, and water. This system is highly non-ideal due to the presence of polar components with hydrogen bonding. The non-ideal nature of the system directly affects the VLE calculations. In this paper, the effect of VLE data on the simulation results has been analyzed using two specially chosen activity correlations: the UNIFAC model and the NRTL equation. A comparison between measured and calculated liquid compositions using these liquid activity models is provided in Fig. 7 for each component. The results are obtained by using the effective mass transfer NEQ model. Clearly, the disagreement between experimental data and simulation results obtained by the UNIFAC equation is considerable. However, the profiles resulting from the NRTL model show a good agreement with experimental results.

A further comparison between outputs of two liquid activity models is performed based on temperature profiles. The tempera-

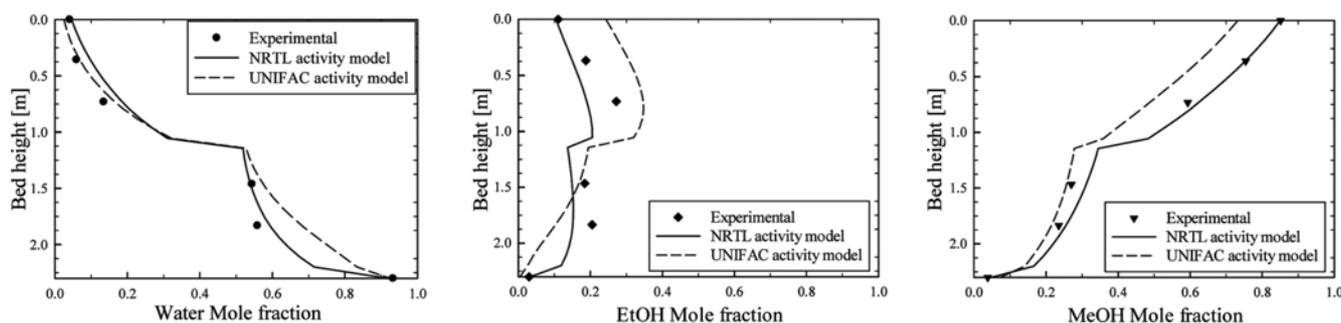


Fig. 7. Liquid composition profiles resulting from the effective mass transfer NEQ model with different activity model in addition to experimental data along the column.

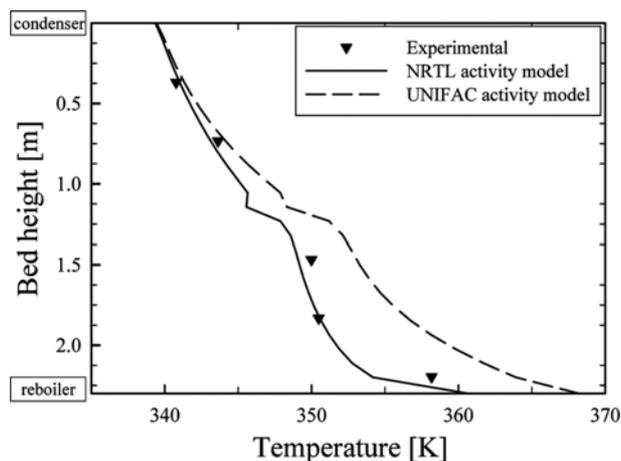


Fig. 8. The temperature profile resulted from the effective mass transfer NEQ model for different activity models in addition to measured temperatures.

ture profiles resulting from NEQ simulations for each activity model are depicted in Fig. 8 where the measurement data along the column are also presented. As is clear in the figure, the temperature profile obtained from the UNIFAC model could not predict the measured data while simulation results from the NRTL model have good agreement with experimental data. Therefore, it can be said that the NRTL equation is the appropriate model for VLE calculations to simulate the mentioned column.

3. The NEQ Model

According to the obtained results for the proper number of packing segments and the appropriate model of liquid activity coefficients, a detailed comparison between simulation results of each NEQ model was performed. Our investigations confirm that the chosen number of segments and activity model are also adaptable for the simulation of random packed column in case study II. Therefore, the results for both packed columns are presented in the following figures. These results were obtained from both NEQ models in addition to results of HETP-based EQ modeling approach. The average HETP value obtained from evaluation of HTU matrix along

Table 6. The quantitative comparison of temperatures between simulation results and experimental data for structured packed column (case study I)

h [m]	Exp.	NEQ 01	(%e)	NEQ 02	(%e)	EQ	(%e)
0.37	340.78	341.34	0.16	340.55	-0.07	342.05	0.37
0.73	343.63	343.87	0.07	343.08	-0.16	343.62	0.00
1.47	349.99	350.43	0.13	350.37	0.11	350.37	0.11
1.83	350.49	352.34	0.53	351.92	0.41	351.95	0.42
2.20	358.18	356.50	-0.47	355.18	-0.84	355.08	-0.86
% Mean relative error			0.27			0.32	0.35

NEQ 01: Non-equilibrium modeling based on effective mass transfer coefficients

NEQ 02: Non-equilibrium modeling based on packing efficiency

EQ: Equilibrium modeling based on HETP concept

the bed height is 25 cm for the mentioned structured packed column, and 12.85 cm for the considered random packed column.

Fig. 9(a), (b) show the temperature profiles and the liquid composition profiles of each component along the column height resulted from the simulation of structured packed column in case study I. In this figure the measurement points taken along the packed bed are also presented.

The temperature profiles (Fig. 9(a)) show that all modeling approaches can predict the measured temperatures precisely. The quantitative comparisons given in Table 6 confirm this where the maximum average discrepancy is less than 0.5%. As shown in Fig. 9(a), the predicted profiles from all modeling approaches are almost similar though a slight difference is seen at the feed position.

The detailed investigation in Fig. 9(b) denotes that the efficiency-based NEQ model predicts the measured compositions more precisely, especially for water and methanol, while the NEQ model based on effective mass transfer coefficients could only predict the composition of methanol in enriching section somewhat better. The predictions of both NEQ models show some deviations relative to experimental data for ethanol in enriching section. It is noticeable that the profiles resulting from EQ modeling approach

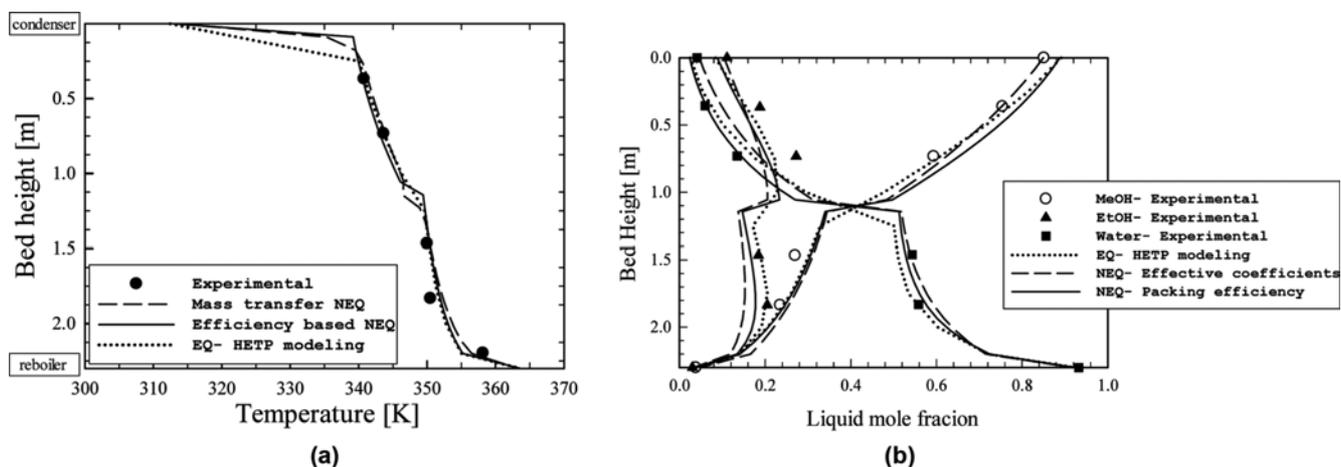
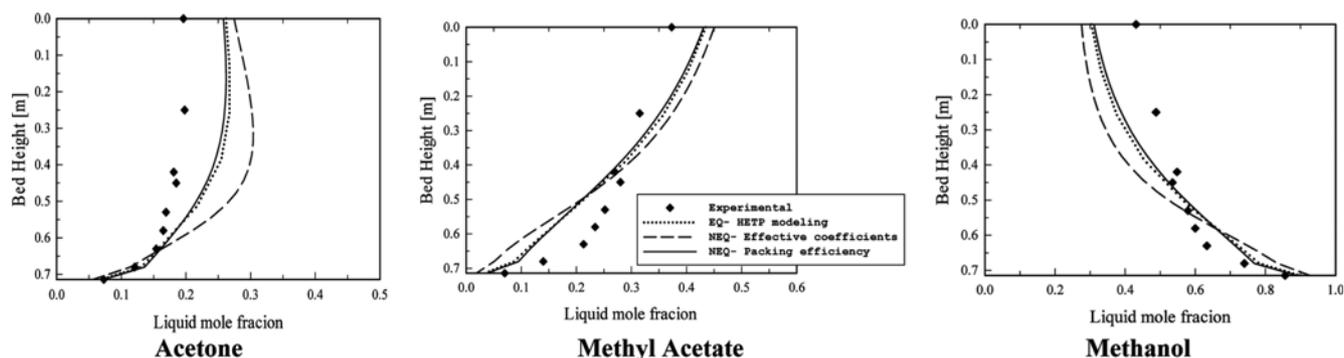


Fig. 9. The obtained profiles from simulation of structured packed column in addition to experimental data. (a) The temperature profiles. (b) The liquid composition profiles.

Table 7. The quantitative comparison of liquid compositions between simulation and experimental results for structured packed column (case study I)

MeOH								EtOH								Water									
h [m]	Exp.	NEQ 01	(%)e	NEQ 02	(%)e	EQ	(%)e	h [m]	Exp.	NEQ 01	(%)e	NEQ 02	(%)e	EQ	(%)e	h [m]	Exp.	NEQ 01	(%)e	NEQ 02	(%)e	EQ	(%)e		
Cond.	0.85	0.849	-0.3	0.886	4.1	0.891	4.7	Cond.	0.11	0.104	-5.6	0.088	-20	0.084	-24	Cond.	0.04	0.047	15	0.025	-38	0.025	-39		
0.36	0.75	0.754	0.0	0.791	4.8	0.771	2.2	0.36	0.19	0.147	-22	0.143	-24	0.156	-17	0.36	0.06	0.096	62	0.064	7.3	0.071	18		
0.73	0.59	0.627	5.6	0.651	9.6	0.609	2.6	0.73	0.27	0.187	-31	0.201	-26	0.220	-19	0.73	0.13	0.185	38	0.148	10	0.171	27		
1.47	0.27	0.321	19	0.310	14.7	0.299	11	1.47	0.18	0.152	-18	0.173	-6.0	0.186	1.2	1.47	0.54	0.526	-3.1	0.517	-4.9	0.515	-5.2		
1.83	0.23	0.262	11	0.248	5.6	0.241	2.7	1.83	0.20	0.155	-25	0.182	-11	0.202	-1.6	1.83	0.56	0.583	4.3	0.568	1.8	0.556	-0.4		
Reb.	0.04	0.048	26	0.040	5.9	0.039	3.1	Reb.	0.03	0.033	9.3	0.036	20	0.037	24	Reb.	0.93	0.919	-1.4	0.924	-0.9	0.924	-0.9		
% Mean error			10.5	7.5			4.4	18.3			17.9			14.5			20.5			10.5			15.2		

**Fig. 10. The liquid composition profiles obtained from simulation of random packed column in addition to experimental data (case study II).**

approximately similar to the NEQ models. This originates from this fact that the HETP value for the considered structured packed column is accurately estimated.

The quantitative comparisons between predicted and measured compositions are separately given in Table 7. The average discrepancies are also given in this Table. It is obvious that the accuracy of both the efficiency-based NEQ model and also HETP-based EQ model is almost the same.

Fig. 10 displays the variation of liquid mole fraction separately for each component along the random packed column in case study II. Simulations were performed based on pseudo-continuous method so that the internal flow rates in the calculations corresponded to experimentally measured value at total reflux operation of column (0.019 mol/s). As seen, the trend of variations is fairly predicted by simulation methods, especially by efficiency-

based NEQ method and HETP-based EQ method. According to the effective mass transfer coefficient method, the prediction of NEQ approach is accompanied by considerable departure relative to measurement data, particularly for acetone. This reveals that the overall mass transfer coefficient has not been acceptably estimated by effective mass transfer coefficients for mentioned non-ideal mixture.

A detailed comparison between simulation and measurement data is given in Table 8. As clearly observed, the simulation with efficiency-based NEQ model has the lowest difference with experimental data, though the discrepancy of results obtained from HETP-based EQ model is almost similar to the efficiency-based model.

Note that the predictions based on all simulation models are accompanied by some deviations relative to experimental results. A source of these deviations can be related to simplifying assump-

Table 8. The quantitative comparison of liquid compositions between simulation and experimental results for random packed column (case study II)

Acetone								Methyl acetate								Methanol									
h [m]	Exp.	NEQ 01	(%)e	NEQ 02	(%)e	EQ	(%)e	Exp.	NEQ 01	(%)e	NEQ 02	(%)e	EQ	(%)e	Exp.	NEQ 01	(%)e	NEQ 02	(%)e	EQ	(%)e				
Cond.	0.196	0.274	40	0.258	32	0.262	34	0.373	0.450	21	0.431	16	0.435	17	0.431	0.275	-36	0.311	-28	0.303	-30				
0.25	0.198	0.302	52	0.260	31	0.268	35	0.315	0.374	19	0.352	12	0.360	14	0.488	0.324	-34	0.388	-20	0.372	-24				
0.42	0.181	0.295	63	0.239	32	0.248	37	0.27	0.277	2.6	0.263	-2.6	0.271	0.2	0.548	0.428	-22	0.498	-9.1	0.481	-12				
0.45	0.185	0.287	55	0.231	25	0.241	30	0.28	0.254	-9.4	0.244	-13	0.251	-10	0.535	0.459	-14	0.524	-2.0	0.509	-4.9				
0.53	0.169	0.249	48	0.206	22	0.209	24	0.252	0.181	-28	0.191	-24	0.192	-24	0.579	0.569	-1.7	0.604	4.3	0.599	3.5				
0.58	0.165	0.210	27	0.184	12	0.182	10	0.234	0.133	-43	0.158	-33	0.153	-35	0.6	0.657	9.5	0.658	10	0.666	11				
0.63	0.154	0.162	5.4	0.161	4.2	0.156	1.4	0.213	0.087	-59	0.124	-42	0.118	-44	0.633	0.751	19	0.715	13	0.725	15				
0.68	0.121	0.114	-5.6	0.136	12	0.131	8.2	0.14	0.051	-63	0.095	-32	0.087	-38	0.74	0.835	13	0.769	3.9	0.782	5.6				
Reb.	0.073	0.056	-23	0.073	-0.5	0.069	-5.9	0.07	0.019	-73	0.038	-46	0.034	-51	0.856	0.925	8.1	0.890	3.9	0.897	4.8				
% Mean error			35.5	19.0			20.6	35.4			24.4			25.9			17.4			10.5			12.2		

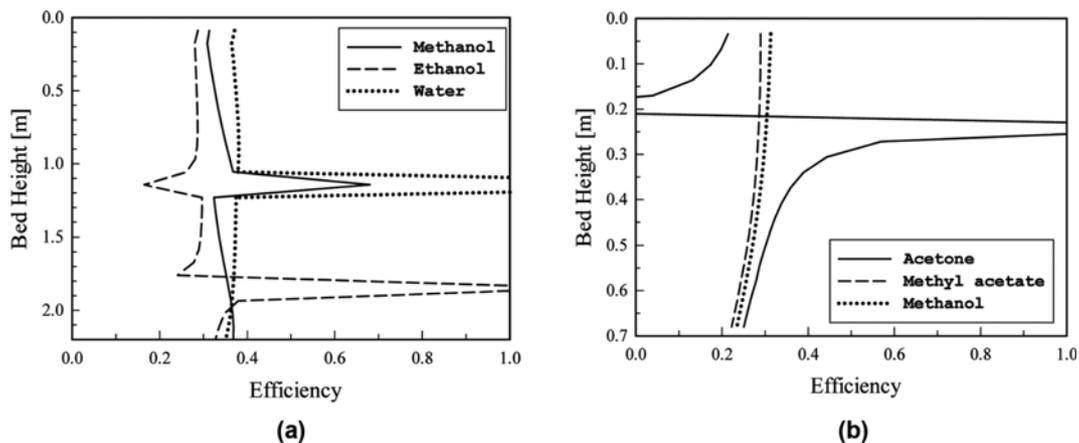


Fig. 11. Estimated efficiencies for different components as a functions of the packing height. (a) The structured packed column (case study I). (b) The random packed column (case study II).

tions applied to develop simulation methods. However, the non-uniform distribution of local fluid flows in different cross-sections of the column is also accounted as another source of the discrepancy of simulation results with experimental data. In fact, in packed columns, particularly with large diameters, some uneven distribution of temperature and component concentrations may have arisen into the column. This issue could affect on the separation efficiency of the mixture and consequently on final results of the simulation [45–49].

In Fig. 11, the estimated component efficiencies for both packed columns are displayed as a function of the packed height for 25 segments. These efficiency values are introduced to the efficiency-based NEQ model for correcting the mass transfer in each segment. According to this, the temperature and composition profiles are obtained. As observed, some component efficiencies change along the packed beds. This means that some components can have different mass transfer characteristics along the columns. Furthermore, in both columns, oscillations are observed in component efficiencies at different sections of each column due to fluctuation of compositions.

CONCLUSION

The separation performance of two multicomponent packed distillation columns, a structured packed column and a random packed column, was simply evaluated using a developed NEQ modeling approach. Non-idealities of the distillation process due to inter-phase mass transfer effects were evaluated by the estimation of mass transfer rates for each phase. The rates of mass transfer were determined using the overall mass transfer coefficients as simple, on-hand method. We proposed distinct estimation methods to obtain the overall mass transfer coefficients, including the effective mass transfer method and the packing multicomponent efficiency method. In this way, we could simulate both packed distillation columns with NEQ effects in a similar structure to EQ stage model. A developed MATLAB home-code was used to implement the simulation algorithms. For modeling, the packed height was divided into a number of segments and the overall mass transfer coeffi-

cients were determined for each segment. Results of temperature and composition profiles were thus obtained and then compared with the experimental measurements from each packed column.

The size of packing segments as an effective parameter in the simulation procedure was investigated in the first step. The comparison of different simulation results with various segment sizes and experimental data for the structured packed column showed that 25 segments are a proper choice for further simulations. In the next step, the non-ideality of liquid mixture separated in the structured packed column was investigated based on two liquid activity models, including the UNIFAC model and the NRTL model. A comparison between measured and calculated profiles using these liquid activity models showed that the NRTL model could predict experimental results more precisely than the UNIFAC model, and so this model was considered as a base for further simulations. Our considerations illustrated that these choices for number of segments and liquid activity model are also adaptable for the simulation of random packed column in case study II. Finally, the results of each NEQ model were compared with the experimentally measured data. For further comparisons, the results obtained from so-called HETP-based EQ model are also presented. The detailed comparisons revealed that the efficiency-based NEQ model had a better agreement with experimental results. However, the accuracy of the EQ model is almost equivalent to efficiency-based NEQ model, due to precise estimation of HETP values for each packed column. The quantitative comparisons showed an acceptable agreement between predicted and measured concentrations along the columns, so that the maximum average difference obtained by efficiency-based NEQ model was about 18% and 25% for the structured packed column and the random packed column, respectively.

By applying the efficiency-based approach, it was possible to evaluate the mass transfer characteristics of each component along the packed bed as packing efficiency values. These efficiency values were successfully incorporated into the mass transfer models to predict the temperature and composition profiles along packed columns. Accordingly, it can be concluded that our simple NEQ approach provides a reliable way to estimate the performance of

real packed columns.

NOMENCLATURE

a_e : effective interfacial area [m^2/m^3]
 a_p : apparent specific surface area [m^2/m^3]
 a_j : interfacial area of segment j [m^2/m^3]
 A_c : column surface area [m^2]
 c^p : molar concentration for each phase [gmol/cm^3]
 c : the number of components
 D^p : diffusion coefficient for each phase [m^2/s]
 d_{eq} : equivalent diameter of a channel [m]
 $(E^{MV})_j$: vector of Murphree segment efficiencies
 E^{MV} : Murphree vapor phase segment efficiency
 $f_{i,j}^p$: component feed flow rate for each phase [mol/s]
 h_j : hsegment height [m]
 H_j : enthalpy [J/mol]
 $[H^{OV}]$: matrix of overall HTUs [m]
 $[H^p]$: matrix of HTUs for each phase [m/s]
 (J^V) : vector of vapor diffusion fluxes [mol/($\text{m}^2\cdot\text{s}$)]
 j : the corresponding stage number
 $[K]$: matrix of vapor-liquid equilibrium constants (K-values)
 $K_{i,j}$: vapor-liquid equilibrium constant
 $[K^{OV}]$: the matrix of overall mass transfer coefficients [m/s]
 $K_{i,j}^{OV}$: overall mass transfer coefficient [m/s]
 $k_{i,j}^p$: binary mass transfer coefficient for each phase [m/s]
 $\kappa_{i,j}^p$: effective mass transfer coefficient for each phase [m/s]
 L_j : liquid flow rate [mol/s]
 $l_{i,j}$: component liquid flow rate [mol/s]
 Q_j : heat load [J/mol]
 r_j^p : side-stream flow rate for each phase, dimensionless
 RR : reflux ratio
 $[R^p]$: inverse matrix of mass transfer coefficients for each phase, dimensionless
 Re : Reynolds number, dimensionless
 S : corrugation spacing [m]
 Sh : Sherwood number, dimensionless
 Sc : Schmidt number, dimensionless
 u_{Ve} : effective vapor velocity [m/s]
 u_{Le} : effective liquid velocity [m/s]
 u_{SV} : superficial vapor velocity [m/s]
 u_{LV} : superficial liquid velocity [m/s]
 V_j : vapor flow rate [mol/s]
 $v_{i,j}$: component vapor flow rate [mol/s]
 v_j : volume of a packed segment [m^3]
 W : bottom product flow rate
 $x_{i,j}$: actual liquid mole fraction
 $y_{i,j}$: actual vapor mole fraction
 $y_{i,j}^*$: vapor composition in equilibrium with $x_{i,j}$
 z_i : mole fraction of the appropriate phase
 ρ^V : vapor density [kg/m^3]
 μ^V : vapor viscosity [Pa·s]

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