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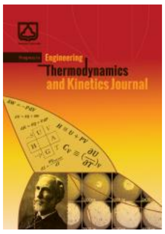

Research Article

A packed distillation column performance simulation by modified equilibrium stage model based on multicomponent packing efficiencies

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ABSTRACT

In this work, a modified equilibrium approach based on the calculation of multicomponent efficiencies is implemented for simulating packed columns. In this modified approach, the non-idealities of the distillation process due to interphase mass transfer are taken into account, while the algorithm remains simple and efficient.The whole method consists of a segment-wise procedure, which is performed iteratively in a computational MATLAB code to simulate an experimental packed distillation column with structured packings. In each iteration, the component efficiencies are determined to consider mass transfer effects through the packed segments. According to the obtained profiles for temperature and component compositions, good agreement is observed between the reported experimental data and simulation results, with average deviations of approximately 0.5% and 19% for temperature and compositions, respectively. This confirms that the modified equilibrium model presented here can accurately predict the performance of multicomponent distillation in packed columns, and therefore it can be employed as a valid and reliable approach for the design and simulation of real distillation towers.

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1. Introduction

For more than a century, researchers have focused on distillation as a significant unit operation for various applications [1]. This process is the most widely practiced method to separate mixtures of chemical species in the petroleum, natural gas, chemical, and petrochemical industries [2]. The distillation process is an energy-intensive method used in many industries to separate compounds based on differences in volatility [3]. Distillation columns are mainly categorized into trayed-type and packed-type columns. Trayed towers are favored when the velocity of the liquid is low, whereas columns with random packings are efficient for high velocity of the liquid. Besides, the structured packings are preferred when the pressure drop is considered as a significant factor. Additionally, they serve as a suitable alternative to trays when a higher degree of separation or capacity is required [4]. According to these advantages, attention to the structured packed towers has increased significantly in retrofitting or improving the existing stage columns [5].

Distillation towers may consume more than half of the plant's energy requirements and thus account for a significant portion of the project's capital costs [6]. Due to high installation capacity and energy usage, distillation has a central effect on the overall performance of industrial plants. Due to the high capital and operating costs of distillation towers, it would be beneficial to utilize mathematical modeling tools for optimizing column operating and design parameters simultaneously, with the aim of minimizing costs.

However, engineers typically design distillation columns based on experience and heuristics, aided by rigorous stage-by-stage distillation models available in commercial process simulation software [7]. An example can be seen in the work by Dai et al. [8], where the economic assessment and optimization of different strategies for ethanol-water azeotrope separation are performed using Aspen Plus. Another recent work by Margarida et al. [9] has used Aspen Plus to optimize a process consists of distillation towers for ethanol recovery and reactive distillation towers for conversion of the residual free fatty acids.

Hence, many researchers have tried to use modeling and simulation tools for optimizing the distillation process. A reliable model is important for evaluating the process performance. Since the control, management, and operation of the distillation columns are accompanied by various complexities, computer programs that adequately describe this operation should be available throughout the industrial plant.

The two main modeling approaches used in distillation design are the equilibrium stage model and the rate-based model (known as the non-equilibrium model) [10]. Both methods use rigorous Mass, Equilibrium, Summation, and Heat or enthalpy relations (MESH) at each stage. In the equilibrium stage model, it is assumed that the liquid and vapor streams from each stage reach the thermodynamic equilibrium. This means that the vapor and liquid phases have the same chemical potential and equal pressure and temperature. This modeling approach does not require detailed design information. It needs only the data for calculating of equilibrium constants and enthalpies. The equilibrium modeling approach is a conventional method for simulating packed distillation towers. Therefore, the packed distillation column is modeled like a staged column, so that the height of the packed bed is divided into several sections, each of which is considered as a separate stage. Here, the balance equations for any packing sections are identical to the corresponding equations for a single stage in trayed columns [11].

Actually, the equilibrium modeling approach can be used together with the Murphree efficiency method for trayed columns and the HETP (height equivalent to a theoretical plate) method for packed towers [12]. These two concepts attach the equilibrium approach to actual equipment design, as the output streams from a stage may not reach thermodynamic equilibrium in practice. A distillation column is more accurately described by the rate-based approach than by the equilibrium method, because it considers the interphase mass transfer between two phases under the assumption that the vapor-liquid equilibrium (VLE) is established only at the interfaces. Unfortunately, this increase in accuracy is dependent on the model size, so that increasing the number of elements will significantly increase the computational load. The equilibrium stage method remains suitable and widely used, representing the thermodynamic limit of the distillation process based on rigorous MESH calculations, even though it may not be as accurate as the rate-based method. Furthermore, it is also satisfactory for conceptual designs and optimization goals.

In fact, in an actual distillation operation, the output streams of a packed section or an actual tray are rarely in equilibrium. To overcome the discrepancy of the model with the actual situation and consequently consider the mass transfer effects, the first solution is to apply the efficiency concept into the equilibrium modeling approach. Accordingly, the deviation from the ideal state on any tray or packing section is accounted by introducing efficiency values into equilibrium relations. Indeed, efficiencies are often used to fit the results of the equilibrium stage model with actual column operating data [13]. For designing a large-scale distillation column, the knowledge of distillation efficiencies and the ability to estimate accurate efficiencies are significant [14]. Efficiencies have a direct effect on the number of required stages and an indirect impact on the equipment running costs. Therefore, the appropriate application of the efficiency concept results in significant savings in capital and operational costs for the distillation process. Additionally, predicting the column efficiency is crucial to determine its performance and meet the desired purity requirements [15]. Therefore, any factors that cause a decrease in efficiency will undoubtedly affect the entire column's performance. So, it is essential to correctly predict the efficiencies before the construction or installation of distillation columns. It can be said that the increase of the separation efficiency, as well as its estimation, has been the main task in the design and operation of distillation columns [16].

HETP concept for packed towers is used as a concept something similar to the stage efficiency in trayed towers. HETP is simply used into equilibrium modeling approach. According to this concept, the separation efficiency of a packed distillation tower is characterized for design purposes. In fact, the mass transfer efficiency of packed distillation columns is defined by HETP concept. Since the mass transfer efficiency of components in binary mixtures is similar, the HETP value of both components is equal.

However, in multicomponent mixtures, HETP values of various components are different as the HETP depends on several factors such as components of the mixture, physical properties of the system, and operating conditions of the column. Therefore, this concept is not directly applicable to multicomponent distillation.

In conventional approaches for the modeling of multicomponent distillations, the efficiency of HETPs is often assumed to be equal for all components in each stage or packed section. However, it has been experimentally demonstrated that in multicomponent distillations, efficiencies can vary from stage to stage and even from component to component [17-19]. As the component efficiencies differ, the same separation would not be obtained using the assumption of constant efficiencies, and consequently, introducing multicomponent efficiency calculations into the modeling algorithm is desirable. If the individual component efficiency could be estimated during the simulation, the design of the column would be significantly improved by avoiding unnecessary over-sizing. Thus, capital and operational costs would be diminished. To the best of our knowledge, none of the commercial simulation programs are capable of handling multicomponent efficiency calculations. Non-equilibrium simulators, such as RateFrac in Aspen Plus [20] and ChemSep [21], can only calculate efficiencies based on the results of non-equilibrium simulations.

In recent years, various researchers have attempted to use multicomponent efficiencies, along with equilibrium modeling, to account for the non-ideality of the distillation process. Aittamaa [22] initially applied the multicomponent efficiency calculations in the distillation modeling.

Later, Ilme [23] developed this approach further. Several researchers, such as Klemola [24] and Jakobsson [25], comprehensively examined this method. Ilme et al. [18] and Jakobsson et al. [19] also applied efficiencies on the modeling of industrial columns. In our previous work [26], a simple non-equilibrium method based on rigorous efficiency calculations was also presented. Schubert et al.[27] present a comprehensive review of the existing theoretical efficiency prediction models along with the critical analysis of their strengths and weaknesses. The future of the tray efficiency modeling is expected to feature hybrid approaches, i.e. using theoretical models accompanied with fluid dynamics information from experimentally validated CFD models.

So far, most of studies conducted to multicomponent efficiency computations have been related to tray distillation columns, and the packed towers are rarely modeled based on this method. Among various researches, Keskinen et al. [28] focused on the equilibrium stage model with multicomponent efficiency factors, and applied it for modeling of packed distillation columns at total reflux conditions. However, they believed that the applied method still requires further verification with additional laboratory data. The primary challenge in packed distillation modeling based on the efficiency approach is determining component efficiencies for any packed section. Furthermore, their application to the simulation and design procedure is not clearly revealed.

This paper aims to discuss the main characteristics of applying a rigorous efficiency-based distillation model to simulate packed distillation columns, with a focus on temperature and composition profiles. This paper also provides a detailed comparison between the efficiency-based mass transfer model and experimental data from a packed distillation column. During the column simulation, individual component efficiencies are estimated for the packed column in question, and then the obtained efficiencies are directly applied in the simulation procedure.

The main characteristic of the presented model is that the multi-component segment efficiencies are simultaneously calculated along with the complete distillation model. Subsequently, the distillation process non-ideality due to mass transfer phenomena is accounted for while the structure of the equilibrium stage model is retained.

2. Model description

Basically, there are two main approaches proposed for modeling of packed columns: discrete approach and continuous approach. In the first approach, the packed bed as a continuous contact system is divided into some segments so that every segment is approximately considered as a separation stage in a tray tower. On the other approach, differential balance equations are explored for a small packing element. Therefore, a numerical integration scheme is applied to solve these differential equations [29, 30]. In present work, the first approach is used so that the packed column is divided into some separate segments. Then, each of them is considered a discrete stage, taking into account their non-ideal behavior. In the model, non-ideal behavior resulting from deviations from the equilibrium state assumption is considered based on multicomponent efficiency calculations. To determine the efficiency of a packed column with mass transfer effects, one mass transfer stage should be initially defined. This requires the packed bed to be vertically discretized into several control volumes, known as segments, each of which contains both vapor and liquid phases with homogeneous composition and temperature. The model equations are then written for each segment. The configuration of a typical segment in the packed column is schematically shown in Figure 1.

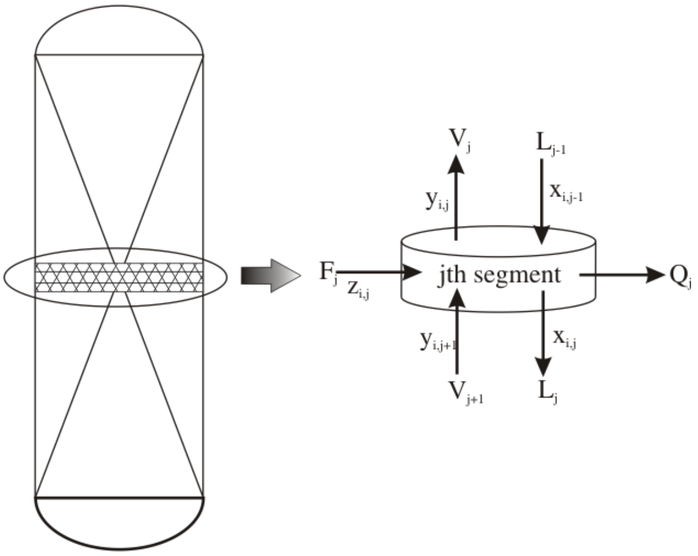

Figure 1. Schematic representation of a segment in the packed column

The equilibrium constants (K-values) are adjusted away from the thermodynamic equilibrium value when the efficiency-based equilibrium model is applied for the evaluation of the column non-ideal behavior. This modification is performed by incorporating the phenomena occurring in the packed bed (such as back-mixing) into a model for K-values.

In contrast, the structure of the ideal stage model is preserved. This approach is inspired by the application of efficiency concept. Several types of efficiencies have been used in the modeling of distillation process, including Murphree [31], Hausen [32] and vaporization [33] efficiencies, with the Murphree efficiency known as the most widely used concept in the distillation column simulations. All of these different types of efficiencies attempt to determine the deviation of real stages from the equilibrium state.

In the procedure of modeling, the whole packed bed is considered as a sequence of mass transfer stages, each of which corresponds to a special height of packing that represents a calculation segment. This segment height is then associated with a mass transfer stage by definition of multicomponent efficiencies. Each segment is numbered from the top to the bottom. The model governing equations, according to Figure 1, are presented in Table 1.

Table 1. Equations of the efficiency-based modified equilibrium model for the jth segment

Material balance equations $v_{i,j}(1+r_j^V)+l_{i,j}(1+r_j^L)-v_{i,j+1}-l_{i,j-1}-f_{i,j}=0$	c equations
Modified equilibrium equations $E_{ij}^{MV}K_{ij}\left(\frac{l_{i,j}}{\sum_{k=1}^{c}l_{k,j}}\right)\sum_{k=1}^{c}v_{k,j}-v_{i,j}+\left(1-E_{ij}^{MV}\right)\left(\frac{v_{i,j+1}}{\sum_{k=1}^{c}v_{k,j+1}}\right)\sum_{k=1}^{c}v_{k,j}=0$	c equations
Energy balance equation $H_j^V(1+r_j^V)\sum_{k=1}^{c}v_{k,j}+H_j^L(1+r_j^L)\sum_{k=1}^{c}l_{k,j}-H_{j+1}^V\sum_{k=1}^{c}v_{k,j+1}-H_{j-1}^L\sum_{k=1}^{c}l_{k,j-1}-H_j^F\sum_{k=1}^{c}f_{k,j}+Q_j=0$	1 equation
Total number of equations	2c+1

In this table, c is the number of species, $f_{i,j}$, $v_{i,j}$ and $l_{i,j}$ are the flow rate of components related to feed, vapor and liquid streams, respectively. r_j is the dimensionless side-stream flow rate and H_j is the enthalpy. E_{ij}^{MV} also stands for component Murphree efficiency.

In the simulation method, the first stage (condenser) and the last stage (reboiler) are considered as ideal equilibrium stages. So, equations written for these stages are different from equations of intermediate stages. The equations for the top and bottom stages are represented in Table 2.

Table 2. 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		$\sum_{k=1}^{c} l_{k,1}-RR\sum_{k=1}^{c} v_{k,1}=0$	$\sum_{k=1}^{c} l_{k,N}-W=0$
Equilibrium relation	Partial	$K_{i,1}\frac{l_{i,1}}{\sum_{k=1}^{c} l_{k,1}}-\frac{v_{i,1}}{\sum_{k=1}^{c} v_{k,1}}=0$	$K_{i,N}\frac{l_{i,N}}{\sum_{k=1}^{c} l_{k,N}}-\frac{v_{i,N}}{\sum_{k=1}^{c} v_{k,N}}=0$
	Total	$\sum_{p=1}^{c}\left(K_{p,1}\frac{l_{p,1}}{\sum_{k=1}^{c} l_{k,1}}\right)-1=0\;(bubble\ point\ equation)$ $\frac{l_{i,1}}{\sum_{k=1}^{c} l_{k,1}}-\frac{v_{i,1}}{\sum_{k=1}^{c} v_{k,1}}=0\;\;(\,i=2:c\,)$	

In Table 2, RR is the reflux ratio and W is the bottom product flow rate.

Accordingly, for a packed distillation column consisting of N calculation segments, N (2c+1) non-linear equations are obtained. This value is equal to the number of equations for the equilibrium stage model. So, using this modeling procedure, it is possible to consider the effect of mass transfer on the column performance without changing the structure of the equilibrium modeling approach. These sets of equations are solved simultaneously by the Newton–Raphson iterative method [34] in which successive sets of the output variables are computed. This calculation loop will continue until the sum of squares of discrepancy functions are inclined to the convergence criteria or zero.

2.1. Multicomponent packing efficiencies

For a dilute system in a packed column, the mass balance for the vapor phase could be written in matrix notation as follow [15]:

$$V\frac{d(y)}{dh}=-(J^{V})a_{e}A_{c} \tag{1}$$

where a_e is the effective interfacial area of the packing and A_c is the column surface area. By using the definition of the vector of diffusion fluxes,(J^V), based on the matrix of overall mass transfer coefficients for vapor phase, $[K^{OV}]$, Eq. (2) is achieved:

$$V\frac{d(y)}{dh}=c^{v}[K^{OV}](y^{*}-y)a_{e}A_{c} \tag{2}$$

where y^* is the vapor composition in equilibrium with the composition of the liquid leaving the stage. Based on the definition of the overall heights of transfer units (HTUs) for the vapor phase, equation (2) can be expressed as:

$$\frac{d(y)}{dh} = [H^{OV}]^{-1}(y^{*} - y) \tag{3}$$

In order to determine the vapor composition profile along the column, Eq. (3) should be integrated numerically. To avoid this, Keskinen [28] suggested that the term $(y^{*} - y)$ could be estimated with the arithmetic average value for a certain segment height. This approximation leads to:

$$(y)_j - (y)_{j+1} = h_j\,[H^{OV}]_j^{-1}\left(\frac{[K]_j\,(x)_j + [K]_{j-1}\,(x)_{j-1}}{2} - \frac{(y)_j + (y)_{j+1}}{2}\right) \tag{4}$$

where $(y)_j$ and $(x)_j$ represent the composition vectors of vapor and liquid streams leaving the segment j, and $(y)_{j+1}$ and $(x)_{j-1}$ indicate the composition vectors of vapor and liquid streams entering the segment j. $[K]_j$ and $[K]_{j-1}$ are the diagonal matrix of K-values corresponding to liquid compositions x_j and x_{j-1}, respectively. $[H^{OV}]_j$ relates to the overall HTUs matrix in segment j and h_j is the segment height.

Now, the packed bed efficiencies can be defined similar to the definition of Murphree plate efficiencies as follow:

$$E_j^{MV} = \frac{y_j - y_{j+1}}{y_j^{*} - y_{j+1}} \tag{5}$$

According to Eq. (5), a diagonal matrix $[A]_j$ is defined in which the reciprocals of term $\left(y_j^{*} - y_{j+1}\right)$ are its arrays:

$$[A]_j = \begin{bmatrix} \frac{1}{y_{1,j}^{*} - y_{1,j+1}} & 0 & \cdots & 0 \\ 0 & \frac{1}{y_{2,j}^{*} - y_{2,j+1}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{y_{c-1,j}^{*} - y_{c-1,j+1}} \end{bmatrix} \tag{6}$$

Eventually, the following expression is obtained to calculate each component's efficiency in each segment of the packed column:

$$(E^{MV})_j = [A]_j\,\frac{h_j}{2}\,[H^{OV}]_j^{-1}\left\{[K]_j\,(x)_j + [K]_{j-1}(x)_{j-1} - (y)_j - (y)_{j+1}\right\} \tag{7}$$

Eq. (7) is our main equation during the modeling of the packed distillation column. This equation is applied to consider the deviation from the equilibrium state. The basic term in equation (7) is the matrix of overall HTUs, $[H^{OV}]$, that should be determined before calculating the segment efficiencies.

2.2. The overall HTUs matrix

The diffusion in a multicomponent system is very complex in comparison with the binary systems. In such systems, the diffusion rate of each component is affected by the diffusivity of all components in the mixture[23]. Therefore, the gradient of chemical potential is the driving force in calculations instead of the gradient of concentration [11, 35].

The component efficiencies are estimated based on the two-film theory in conjunction with multicomponent mass-transfer theory, as outlined in Maxwell-Stefan diffusion relationships [15]. In the mass transfer model of packed columns, the correlations of binary mass transfer coefficients are used to obtain the matrices of multicomponent height of transfer units (HTUs) for each phase. Then, the matrix of overall HTUs can be calculated.

These calculations require some data about the geometry of the packed column and packing elements, the internal vapor and liquid flow rates, and the physical properties of each phase. The matrices of HTUs for the liquid and vapor phases are determined as follows:

$$[H^L] = \frac{[R^L]u_{SL}}{a_e} \tag{8}$$

$$[H^V] = \frac{[R^V]u_{SV}}{a_e} \tag{9}$$

Where u_{SL} and u_{SV} are the superficial velocities for liquid and vapor phases, respectively. $[R^V]$ and $[R^L]$ are the inverse matrices of mass transfer coefficients with elements calculated by Eq. (10).

$$\begin{aligned} R_{i,i} &= \frac{z_i}{k_{i,c}} + \sum_{\substack{m=1 \\ m\neq i}}^{c} \frac{z_m}{k_{i,m}} \\ R_{i,j} &= -z_i\left(\frac{1}{k_{i,j}} - \frac{1}{k_{i,c}}\right) \end{aligned} \tag{10}$$

In the above equation, z is the considered phase mol fraction, and $k_{i,j}$ is the binary mass transfer coefficient for the same phase.

Finally, the matrix of overall HTUs is determined using the multicomponent HTU matrices for vapor and liquid phases as follows:

$$[H^{OV}] = [H^{V}] + \frac{V}{L}[K][H^{L}] \tag{11}$$

Here, $[K]$ represents a diagonal matrix consisting of vapor-liquid equilibrium (VLE) constants.

In order to calculate the coefficients of binary mass transfer in Eq. (10), different correlations were presented for various commercial packings. In the present work, the relation of Bravo et al. (1985) [36] for structured packings is applied.

By using this relation, the vapor and the liquid binary mass transfer coefficients are predicted as:

$$k^{V} = \frac{Sh_{V}\, D^{V}}{d_{eq}} \tag{12}$$

$$k^{L} = 2\sqrt{\frac{D^{L} u_{Le}}{\pi\, S}} \tag{13}$$

where Sh_V denotes the Sherwood number, d_{eq} represents the channel equivalent diameter, S is the spacing of corrugation (channel side), u_{Le} is the liquid effective velocity, and D is the diffusion coefficient.

There are also several correlations for the calculation of the effective interfacial area per unit volume (a_e). This parameter is a complex function of various properties and operating conditions. Based on the method proposed by Bravo et al. (1985), the surface is considered completely wet. Hence, the interfacial area density (a_e) is considered equal to the apparent specific surface area (a_P). Consequently, the interfacial area is determined as a product of a_P and the volume of the jth segment.

3. Simulation procedure

To implement multicomponent efficiency calculations for a packed distillation column, a sequence of steps is applied for all segments. The general outline of the segment-wise efficiency calculations is presented in Figure 2.

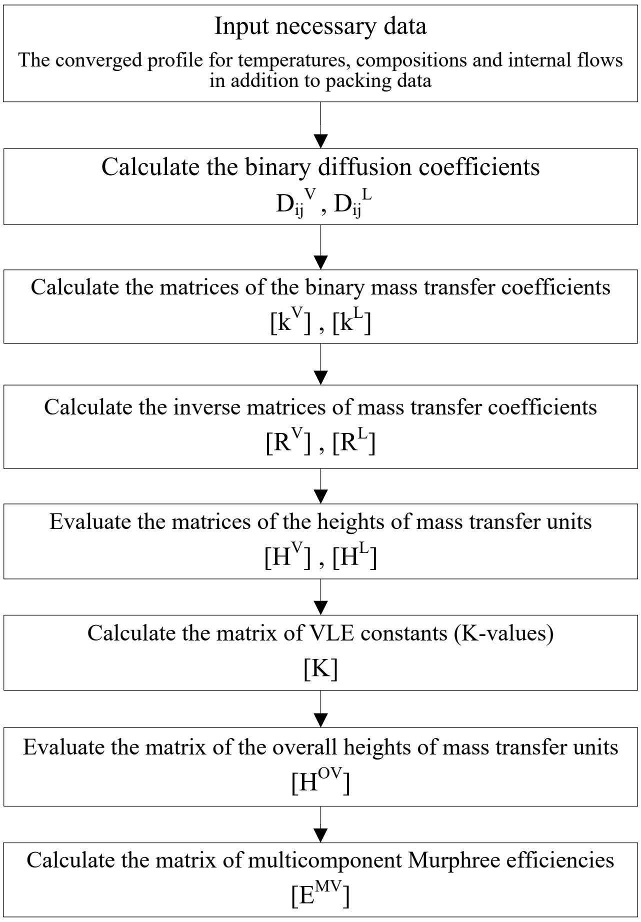

Figure 2. The sequence of multicomponent efficiency calculations for each segment

The whole calculation procedure for the packed column proceeds as follows. The height of the packed bed is initially divided into a number of segments. Next, each segment corresponds to a mass transfer stage by introducing the efficiency values. To accomplish this, segment-wise efficiency calculations, as shown in Figure 2, are implemented in each iteration. Then, the obtained packing efficiencies are applied to correct the compositions at the equilibrium relations. The improved Newton-Raphson approach has been employed to solve the set of equations for the model simultaneously. This pattern is repeated until complete convergence of the mathematical model for the entire packed column. The detail of the modeling method is presented as a flowchart in Figure 3.

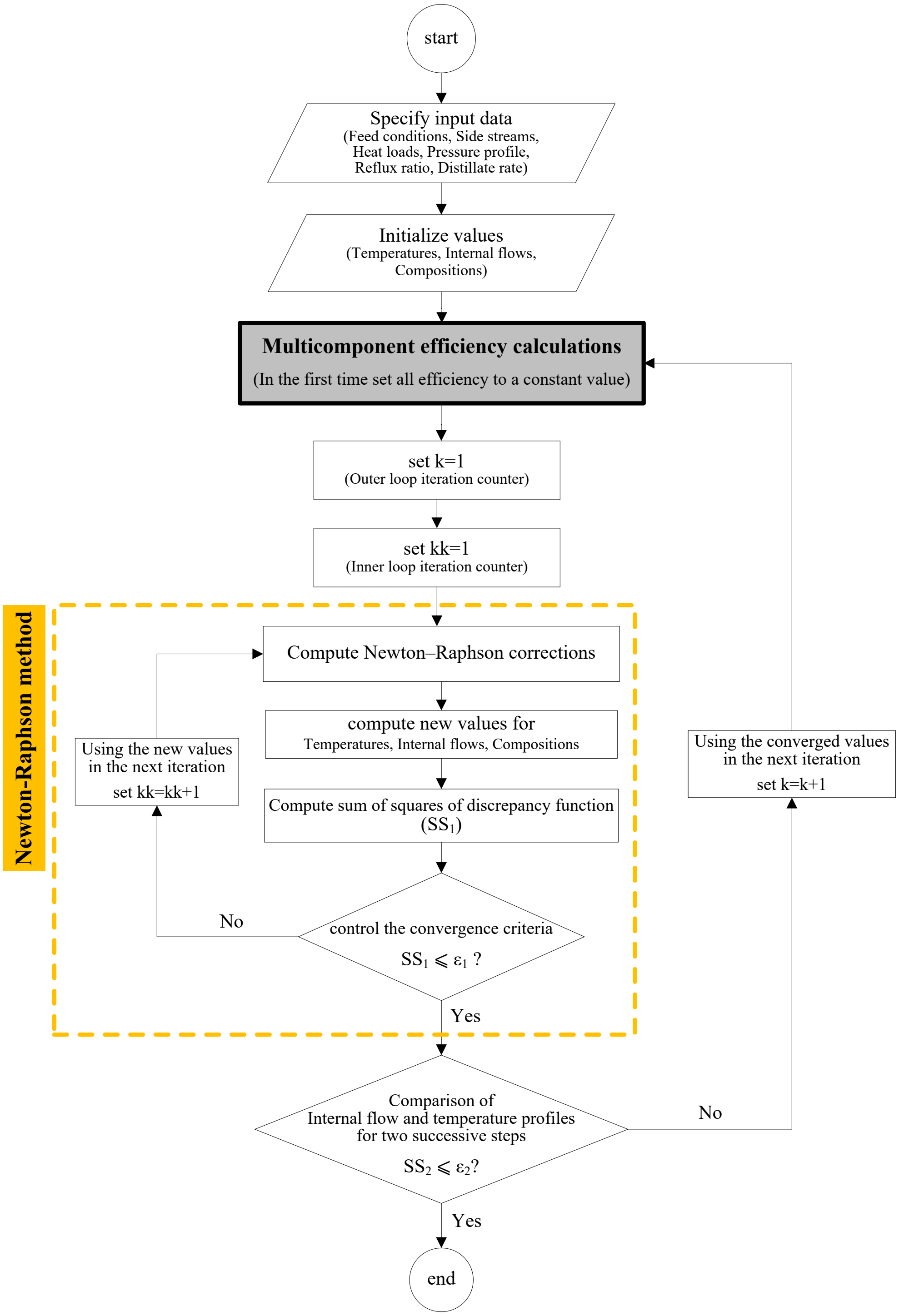

Figure 3. The sequence of whole simulation steps

The simulation model of the column was specified by defining main inputs, including the system thermodynamics, the flow rate, condition, and composition of the feed stream, as well as information about the column and structured packing elements.

Vapor-liquid equilibrium (VLE) calculations are performed based on the $\gamma - \phi$ approach [37]. In this approach, a liquid activity coefficient model is employed to account for the thermodynamic properties of the liquid phase, while an equation of state is used for the vapor phase. In the present work, the NRTL activity model [38] is applied for the liquid phase, and the SRK equation of state [39] is applied for the vapor phase. In addition, the column is assumed to be adiabatic. The NRTL parameters used in this work are presented in Table 3. The provided parameters are used together with $G_{ij} = exp\left(-\alpha_{ij}\tau_{ij}\right)$ and $\tau_{ij} = B_{ij}/T$.

Table 3. NRTL parameters for binary mixtures at 101.3 kPa[40]

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

The modified equilibrium method, along with the calculation of multicomponent packing efficiencies, is executed in a computational code written in MATLAB. This computational code can simulate any packed column with any segment number, including various types and sizes of packings, as well as different column diameters. One of the significant advantages of our developed code is its ease of modification, allowing for the verification of various assumptions. Furthermore, the code has high flexibility to solve convergence issues.

4. Validation method

In this paper, a laboratory-scale packed distillation column (presented by Mori et al. [41]) for the separation of a non-ideal ternary mixture containing methanol, ethanol, and water is considered to evaluate the modeling method. A schematic diagram of the desired packed column is presented in Figure 4. As shown in the Figure, feed enters from the middle of the packed bed. Therefore, the height of the stripping and enriching sections is the same, and each section consists of six structured packing elements. The geometry of the used packings is similar to other commercial corrugated sheet-type packings. However, its sheets are sandwiched by gauze. Therefore, the wetting properties are identical to gauze-type packings. Packed column characteristics and the geometry of the structured elements are specified in Table 4. The operational conditions used in the experiment are also given in Table 5.

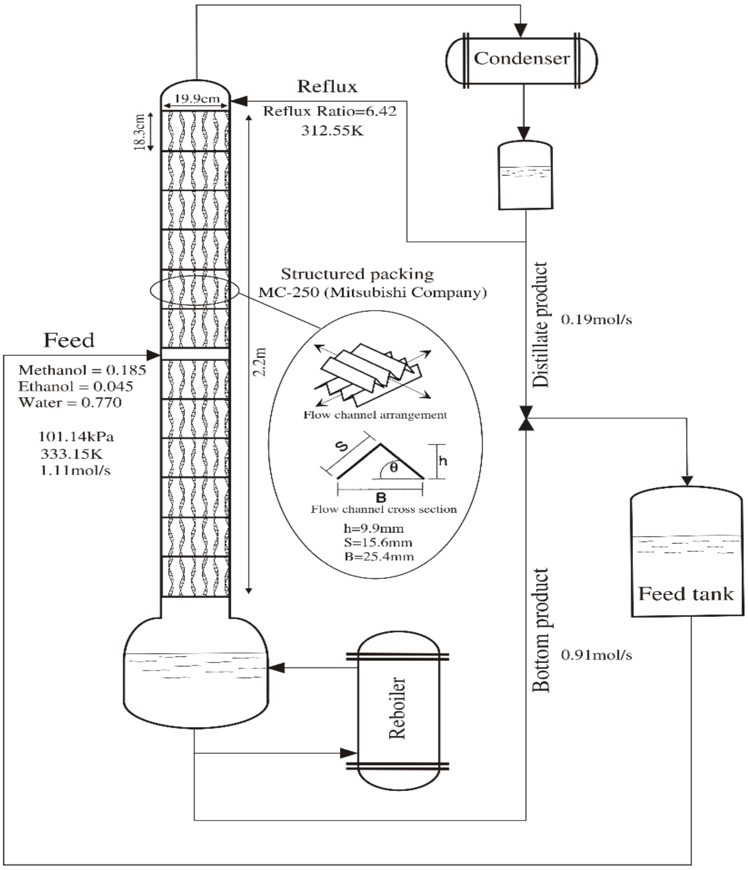

Figure 4. Schematic representation of the packed distillation column, in addition to packing specifications

Table 4. Specifications of the packed column and information on packing elements

Column specifications	
Column height	3 m
Packed height	2.2 m
Diameter	0.21 m
Packing elements information	
type	MC-250 (Mitsubishi Company)
Element diameter	0.199 m
Element height	0.183 m
Height of the triangle	9.9×10^{-3} m
Base of the triangle	25.4×10^{-3} m
Corrugation spacing	15.6×10^{-3} m
Specific surface area	250 m^2/m^3
Void fraction	0.98
Channel flow angle	45°

Table 5. Operating condition of the packed distillation column

specification	**value**	
Reflux ratio	6.42	
Reflux temperature	312.55 K	
Column pressure	101.4 kPa	
Feed flow rate	1.11 mol/s	
Feed composition (mole fraction)	Methanol	0.185
	Ethanol	0.045
	Water	0.770
Feed temperature	333.15 K	
Distillate flow rate	0.19 mol/s	

The physical properties for the mixture and pure components are estimated with several methods presented in Table 6. Moreover, Table 6 presents the relationships used for calculating the binary mass transfer coefficients and the effective interfacial area for the commercial structured packing being used.

Table 6. Methods for estimating physical and mass transfer properties

Physical properties [42]	
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 [Reid et al., 1987]
Mixture gas viscosity	Grunberg and Nissan's 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 Doraisway method
Binary mass transfer coefficient	Bravo et. al. (1985)
Effective interfacial area	equal to the specific packing surface ($a_e = a_p$)

5. Results and discussion

According to the efficiency-based modified equilibrium model presented, a packed distillation column is selected to carry out the simulation procedure. This column separates a ternary non-ideal mixture of methanol, ethanol, and water. The simulations aim to examine the behavior of the desired packed column under operational conditions using the modified modeling method.

To derive the fundamental equation (7) for estimating packing efficiencies, it is primarily assumed that the integral solution of equation (3) is approximated using the arithmetic mean value of the term $y*-y$. It is clear that equation (7) approaches the integral solution as the height of the segments decreases. Therefore, the number of calculation segments significantly affects the precision of the results. Furthermore, segment size directly influences total computation time. Additionally, if the segment height is too small, the segment efficiencies will be quite low. This results in numerical instabilities due to large fluctuations in the model variables, which require more computation time.

Conversely, if the height of the calculation segments is too high, numerical problems may occur during the calculations, leading to a decrease in the accuracy of the obtained results. Understanding suitable segment height can lead to reasonable outcomes. Thus, the effect of the number of calculation segments is thoroughly examined by altering the number of divisions along the packed column.

Figure 5 illustrates the predicted temperature profiles along the column for different segment sizes. Additionally, the measured temperatures along the packed bed are displayed. As expected, the temperature decreases from the bottom to the top of the column. Notably, a significant change occurs at the feed inlet, which becomes more pronounced as the number of segments increases. Figure 5 also demonstrates a strong agreement between the predicted results and the measured temperatures. The quantitative comparisons between the simulation results and the experimental data (for 25 segments) confirm this, as shown in Table 7. The mean relative error for the temperature data is approximately 0.5%.

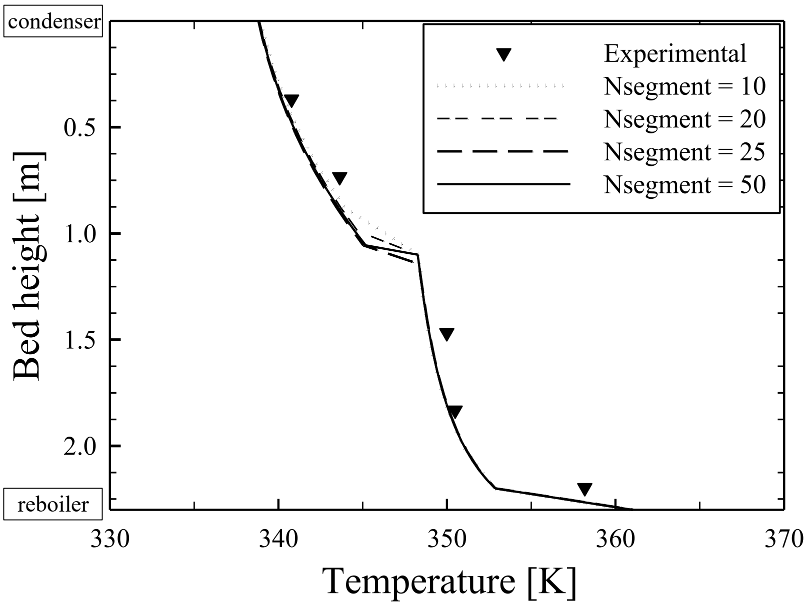

Figure 5. The predicted temperature profiles along the packed height based on several segment sizes.

Table 7. The quantitative comparison between simulation and experimental temperature data (Nsegments=25)

(%e)	T_sim.	T_exp.	h [m]
-0.18	340.2	340.8	0.37
-0.38	342.3	343.6	0.73
-0.29	349.0	350.0	1.47
-0.11	350.1	350.5	1.83
-1.51	352.8	358.2	2.20
	% mean error		

On the other hand, the influence of segment size on predicting column performance is evaluated by comparing each component's composition profile with the measured compositions along the column. Thus, a comparison of predicted liquid compositions for various segment sizes and experimental data is presented in Figure 6. The experimental data consist of four liquid compositions taken along the length of the packed bed. As shown in the figure, the efficiency-based modeling approach effectively predicts the composition of all species. The quantitative comparisons between simulation and measured compositions along the column (25 segments), presented in Table 8, support this conclusion. The primary discrepancy between the plant data and simulation results relates to the concentration of ethanol.

Moreover, Figure 6 indicates that increasing the number of segments can reduce errors in the predicted compositions, especially in the middle of the column. Figure 6 also illustrates that the differences in the profiles between various segment sizes at the top and bottom sections are less pronounced than those in the middle section.

According to the obtained results, the deviation of compositions and temperatures from the experimental data through the packed bed is minimal. Thus, the modified approach is confidently recommended for the design of packed distillation columns.

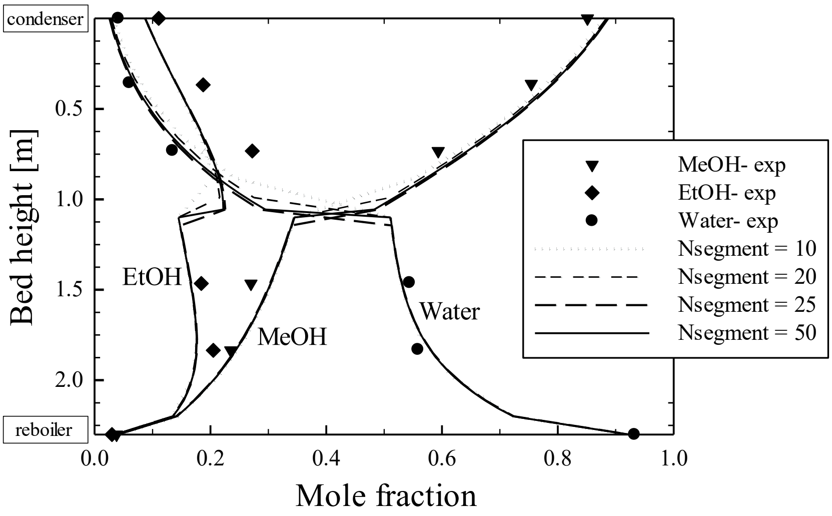

Figure 6. Liquid mole fraction profiles of all components along the packed height for different segment sizes.

According to our findings, increasing the number of segments leads to significant changes in both temperature and composition profiles in the middle section of the column. However, the differences between profiles become less noticeable when the number of segments is greatly increased. Therefore, based on the resulting profiles for various segment sizes, it can be concluded that the simulation with 25 segments (8.8 cm for each segment) is efficient for accurately predicting experimental profiles.

Table 8. The quantitative comparison of liquid compositions between simulation and experimental data (Nsegments=25)

Water			**EtOH**			**MeOH**			**h [m]**
(%e)	Sim.	Exp.	(%e)	Sim.	Exp.	(%e)	Sim.	Exp.	
-41.6	0.02	0.04	-20.4	0.09	0.11	4.3	0.89	0.85	condenser
3.7	0.06	0.06	-23.1	0.14	0.19	5.3	0.79	0.75	0.36
6.8	0.14	0.13	-25.3	0.20	0.27	9.9	0.65	0.59	0.73
-2.9	0.53	0.54	-9.7	0.17	0.18	13.3	0.31	0.27	1.47
3.0	0.58	0.56	-13.4	0.18	0.20	4.8	0.25	0.23	1.83
-0.9	0.92	0.93	20.5	0.04	0.03	5.0	0.04	0.04	reboiler
9.8			**18.7**			**7.1**	**% mean error**		

In Figure 7, the calculated component efficiencies for the packed column under consideration are depicted as a function of the packed bed length for 25 segments. Based on these efficiency values, the mass transfer in each segment is corrected, after which the temperature and concentration profiles are obtained. As shown in Figure 7, the component efficiencies differ from one another. This indicates that each component can have varying mass transfer properties along the column. Furthermore, oscillations in component efficiencies can be observed in the middle section of the column. This is due to fluctuations in the compositions at the feed inlet.

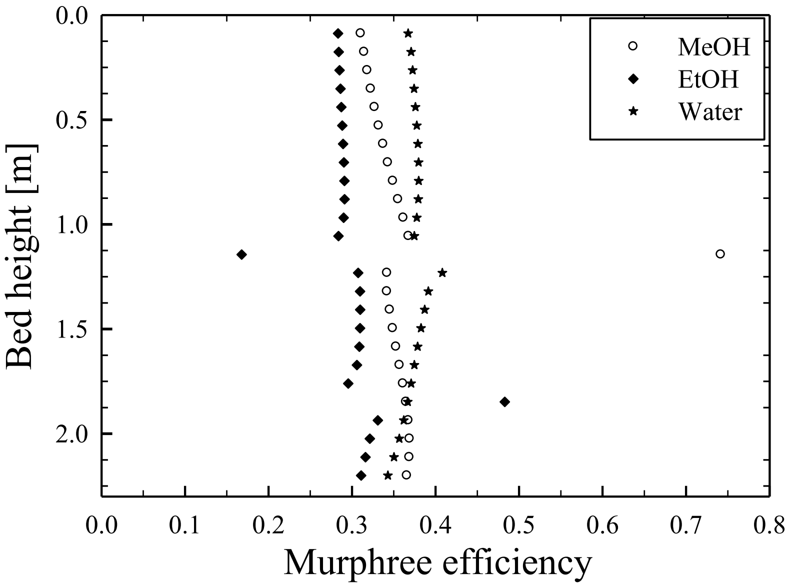

Figure 7. Calculated efficiencies for different components as a function of the packing height

It is important to note that packing efficiencies depend on segment size, resulting in reduced efficiencies as segment size decreases. This indicates that no specific trend for the efficiency profile along the packed bed is expected, unlike trayed columns. In fact, the efficiency profile across the height of a trayed column is unique due to the constant number of stages.

6. Conclusion

A simulation algorithm utilizing an equilibrium model modified by multicomponent packing efficiencies is implemented as a rigorous method for evaluating the performance of packed distillation columns. The main feature of the modified method is its ability to maintain the simple structure of the equilibrium model. In the present model, the non-ideality of a real distillation column, resulting from mass transfer phenomena, is considered through multicomponent efficiency calculations. For modeling purposes, the packed column was divided into separate segments, and the multicomponent efficiencies were determined for each segment. A basic equation was introduced to evaluate the packing efficiencies. To implement the simulation process, an experimental packed column with structured packings to separate a ternary non-ideal mixture was chosen. For validation of the modified approach, the results obtained are compared with reported measurement data. The effect of segment size on the precision of the results was investigated, concluding that simulating with 25 segments can effectively predict the reported experimental data. The qualitative and quantitative comparisons displayed good agreement between the simulation results and the experimental data, so that the average deviations of about 0.5% for temperature and 18% for component compositions were acquired. These results were obtained based on estimated component efficiencies. The resulting efficiency profiles confirmed that each component can have distinct mass transfer characteristics due to differences in component efficiencies along the column.

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Nomenclature

V_j	vapor flow rate, mol/s
$v_{i,j}$	component vapor flow rate, mol/s
L_j	liquid flow rate, mol/s
$l_{i,j}$	component liquid flow rate, mol/s
F_j	feed flow rate, mol/s
$f_{i,j}$	component feed flow rate, mol/s
r_j	the dimensionless side-stream flow rate
y	the vapor mole fraction
y^*	the vapor composition in equilibrium with the outlet liquid composition
x	the liquid mole fraction
z	the mole fraction of appropriate phase
H_j	the enthalpy, J/mol
Q_j	heat load, J/mol
RR	Reflux Ratio
W	bottom product flow rate
h_j	the segment height, m
a_e	the effective interfacial area, m^2/m^3
a_p	the apparent specific surface area, m^2/m^3
A_c	the column surface area, m^2
$[K]$	the matrix of vapor-liquid equilibrium constants (K-values)
$[K^{OV}]$	the matrix of overall mass transfer coefficients, m/s
(J^V)	the vector of diffusion fluxes, $mol/(m^2.s)$
$[H^{OV}]$	the matrix of overall HTUs
$[H]$	the matrix of HTUs for each phase
$[R]$	the inverse matrix of mass transfer coefficients
E^{MV}	Murphree vapor phase segment efficiency
$k_{i,j}$	the binary mass transfer coefficient, m/s
Sh	Sherwood number, dimensionless
D	the diffusion coefficient, m^2/s

d_{eq}	the equivalent diameter of a channel, m
S	the corrugation spacing, m
u_{Le}	the effective liquid velocity, m/s
u_{SV}	the superficial vapor velocity, m/s
u_{LV}	the superficial liquid velocity, m/s

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