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Efficiency estimation of tray columns based on flow profiles and vapor-liquid equilibrium characteristics of binary mixtures

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Abstract: A new systematic approach for estimating the section and column efficiencies based on flow profiles and vapor-liquid equilibrium (VLE) characteristics of binary mixtures exclusively for each tray is proposed. A novel iterative technique for approximating the slope of the VLE curve and the tray efficiency is also developed. For demonstrating the predictive capabilities of the new approach, two case studies are formulated in this work - one with a theoretical column processing selected binary mixtures at total reflux, and the other involving an industrial column whose performance data is acquired from the literature. An in-depth analysis of theoretical column study reveals the superiority of the new approach over the most applied method. In the case study of industrial column, the new approach predicts the section efficiency accurately, unlike the efficiency underestimation from the most applied method. Such an approach would allow a priori calculation of the section and column efficiencies in the tray and column design phase.

1. Introduction

Distillation is the leading separation technology in chemical process industries.[1] It is also likely to lead separations in the future mainly because of two reasons. First, it has distinct economic advantage while processing large throughputs.[2] Second, any alternative to this industrially viable technique is not yet available.[1,3] A recent estimate in 2016 claims that column distillation accounts for 10 to 15% of the global energy consumption.[4] These columns also demand up to 50% of both capital and operational costs in industrial processes.[5] Half of the columns existing worldwide are equipped with cross-flow trays, and this trend is also likely to continue in the future.[6] Among these columns, the most common internals are the single-pass cross-flow trays.[6] In fact, such columns are viewed as cascades of trays with similar geometries and functions.[3] This generalized perspective has prompted numerous experimental and theoretical studies on hydrodynamics and mass transfer efficiency of individual trays. The majority of the existing studies covered the hydrodynamic aspects of sieve trays such as flow capacity, pressure drop, holdup distribution, weeping and so forth.[1] It is known that the tray hydrodynamics are affected by flow maldistribution. However, only few studies investigated the two-phase flow and mixing patterns on these trays through experiments and CFD simulations. Even fewer proposed models for associating these patterns with the Murphree tray efficiency. Such models are based on relationships developed from the analyses of two-phase flow, cross-flow hydraulics and mass transfer over the trays.[7] A collective description of the aforestated experimental and theoretical studies can be found in the literature.[1,3]

Thousands of columns operating worldwide suggest that any improvement in distillation technology could potentially reduce their cost and energy expenditures on a global scale.[1,8] But, to quantify any progress, methods for estimating the overall column efficiency should be at hand. As already mentioned, the prediction of the tray efficiency based on flow and mixing profiles over a single column tray is possible. However, adequate utilization of the individual tray efficiencies in the column efficiency estimation has not been attempted in the literature. In other words, the existing

approaches for the column efficiency prediction do not exclusively consider the individual tray efficiencies governed by flow and mixing profiles and vapor-liquid equilibrium (VLE) characteristics of the mixtures. For supporting the previous assertions, the existing approaches are briefly revisited here. The definition of the overall tray column efficiency is

$$E_o = \frac{N_{eq}}{N} \quad , \tag{1}$$

where N_{eq} is the number of equilibrium stages (obtained using the McCabe-Thiele (MT) method),[9] and N is the actual number of trays in the column.[3] Usually, eq 1 is used for estimating section efficiencies in a column in case there are two or more sections owing to feed and side draw streams. It is allowed to use eq 1 for determining the overall column efficiency, if the whole column is considered as one section.[1] The simplest method for estimating the column efficiency is the O'Connell's correlation,[10,11] which is

$$E_o = 0.503(\mu_L \cdot \alpha_{avg})^{-0.226} \quad . \tag{2}$$

Here, α_{avg} is the average relative volatility of a binary mixture, and μ_L is the liquid viscosity of the feed (in mPa·s), both calculated at the average column temperature. This equation is known to provide conservative estimations that are suitable for preliminary studies only,[1] and to ignore the explicit inclusion of parameters representing the mass-transfer performance.[11] Further, in this correlation, the reason for including the relative volatility over more relevant parameters such as the slope of the VLE line (m) or the stripping factor ($\lambda(=mV/L)$) is also unclear.[1,11] In another study, Lewis[12] forecasted the impact of the tray efficiency on the overall column efficiency as

$$E_o = \frac{\ln\{1 + E_{MV}(\lambda - 1)\}}{\ln \lambda} \quad . \tag{3}$$

In eq 3, it is assumed that the VLE and the operating lines are straight but may not be necessarily parallel along with a constant tray efficiency for each tray.[1] This equation has found application in

the renowned AIChE's bubble-tray design manual.[13] In reality, the stripping factor varies over a column because of the variation of the VLE data and the slope of the operating lines. The stripping factor and the tray efficiency have been assumed as constant over the whole column in eq 3, thus, rendering this method acceptable only for approximate estimations. Recently, Mathias[14] calculated the actual number of trays in a column by resorting to a graphical technique similar to the MT method. In that study, a stepping procedure was followed between VLE and operating lines on an x-y chart based on a fixed tray efficiency, unlike the MT method, where the same procedure is applied for the equilibrium trays (i.e., trays with 100% Murphree efficiency). Assigning a fixed efficiency to each tray for the column efficiency calculation suggests the applicability of this approach for qualitative evaluations only.[14] Further, Górak and Schoenmakers[2] suggested the capacity and efficiency testing of trays during their development stage for identifying potential design problems and subsequent improvements. Schultes[15] confirmed that such practice is non-existent for new trays and emphasized the need for pre-emptive calculations of fluid dynamics and separation efficiency during their development phase. In addition, Taylor[16] acknowledged the necessity of approaches for calculating thermodynamic properties needed in the efficiency models and for modeling the performance of distillation columns. Therefore, a methodical approach is needed for a priori estimation of the section and column efficiencies based on tray-to-tray efficiency calculations governed by flow and mixing profiles and VLE characteristics of the mixtures. Instead, potential areas for improving tray and hence, column performances are currently identified in the post-design phase leading to considerable losses in the industry.[15]

The objective of this work is to formalize a new systematic strategy for evaluating the section and column efficiencies involving flow and mixing profiles on single-pass cross-flow trays and VLE data of binary mixtures. At first, appropriate thermodynamic models are employed for generating the VLE data of the binary mixtures. Liquid flow profiles in the form of residence time distributions (RTD) are assigned to the trays using the axial-dispersion model (ADM). Further, vapor plug flow is

considered through the trays with perfect mixing occurring in the disengagement zones between them. A novel iterative approach is then proposed that considers these information, and computes the slope of the VLE line and the tray efficiency using the standard tray efficiency model. Following the new approach for tray-to-tray efficiency calculations allows obtaining the resultant column efficiency. Two case studies are presented in this work to elucidate the proposed strategy. In the first study, a theoretical column operating at total reflux is considered for selected binary mixtures. In the second study, the same approach is employed for examining real column data acquired from the literature.

2. Case study I

2.1 Column configuration, test systems and VLE data

In the literature, the overall column efficiency is usually monitored for tray columns operating at total reflux (see Figure 1a).[2,13,17,18] In such configuration, all vapor leaving through the column top is fully condensed and routed back to the column as reflux. Further, all liquid leaving through the bottom of the column is vaporized in the reboiler and returned back to the column.[2] This leads to equality between the liquid and vapor molar flow rates (i.e., $L = V$). Such equality is advantageous for estimating the column performance, which is sensitive to the L/V ratio. According to Lockett,[1] inaccuracies in the measured reflux ratio can cause significant errors in the efficiency calculations. The absence of feed and product streams in this configuration further avoids possible feed fluctuations and discrepancies between the feed inlet and feed-tray compositions.[19] On the other hand, the studies with finite reflux are scarce and usually preferred for hydraulic studies only.[2]

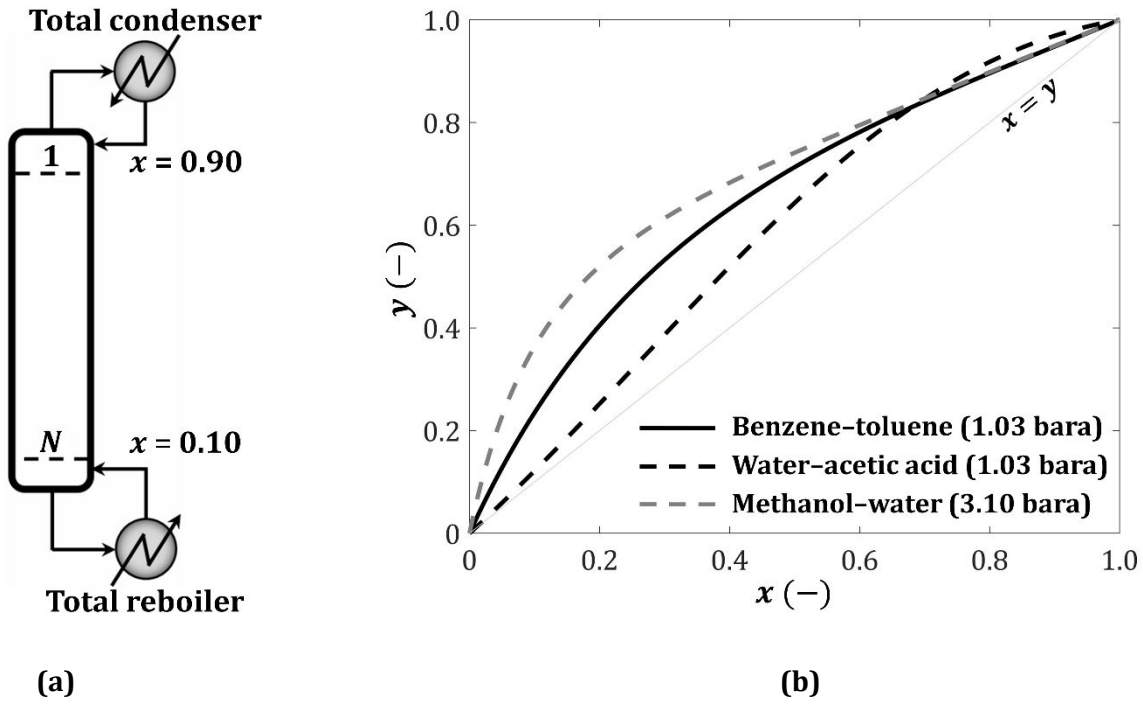


Figure 1. (a) Tray column operating at total reflux mode and (b) VLE plot of standard binary mixtures at given total pressures.

Accurate VLE data are the prerequisites for column performance simulations.[1,2] According to Kister,[18] any uncertainty in such data results in inaccurate tray-to-tray efficiency calculations, particularly for low volatility systems. Many different thermodynamic models exist in the literature for generating physical and thermodynamic properties of the processes, such as Soave-Redlich-Kwong (SRK), Non-Random Two-Liquid (NRTL), Hayden-O'Connel (HOC), Peng-Robinson (PR), Universal Quasichemical (UNIQUAC), and so forth.[15] Recently, De Hemptinne and Ledanois[20] reported a list of criteria (i.e., decision tree) for an appropriate selection of thermodynamic models for industrial applications. Seader et. al[19] also reported a list of industrial binary distillation operations with representative values of the total column pressure. From this literature, the test systems and their representative pressures are derived. Suitable thermodynamic models are selected for these systems based on the earlier mentioned decision tree[20] and other references.[21,22]

Table 1[19] summarizes the selected binary mixtures, column pressures and applied thermodynamic models.

Table 1. Binary mixtures with representative column pressures, thermodynamic models, relative volatilities and minimum number of trays in the column.

Binary mixture	Operating pressure (bara)	Thermodynamic model	α_{avg} (-)	N_{min} (-)
Propylene-propane	19.31	Soave-Redlich-Kwong (SRK)[20]	1.12	37.21
m-xylene-o-xylene	1.03	Soave-Redlich-Kwong (SRK)[20]	1.14	32.58
Vinyl acetate-ethyl acetate	1.03	Non-Random Two-Liquid (NRTL)[20]	1.16	29.43
Isopentane-n-pentane	2.07	Soave-Redlich-Kwong (SRK)[20]	1.26	19.06
Isobutane-n-butane	6.90	Soave-Redlich-Kwong (SRK)[20]	1.30	17.00
Ethylene-ethane	15.86	Soave-Redlich-Kwong (SRK)[20]	1.54	10.19
Methanol-ethanol	1.03	Universal Quasichemical (UNIQUAC)[20]	1.68	7.94
Acetic acid-acetic anhydride	1.03	Non-Random Two-Liquid (NRTL) - Hayden-O'Connel (HOC)[21]	1.73	14.48
Toluene-ethylbenzene	1.03	Soave-Redlich-Kwong (SRK)[20]	1.98	6.54
Water-acetic acid	1.03	Non-random two-liquid (NRTL) - Hayden-O'Connel (HOC)[21]	2.08	9.91
Benzene-toluene	1.03	Soave-Redlich-Kwong (SRK)[20]	2.37	4.88
Propane-1,3-butadiene	8.27	Soave-Redlich-Kwong (SRK)[20]	2.58	4.73
Methanol-water	3.10	Cubic-Plus-Association (CPA)[22]	3.27	3.89
Cumene-phenol	0.07	Universal Quasichemical (UNIQUAC)[20]	4.21	2.75
Benzene-ethylbenzene	1.03	Soave-Redlich-Kwong (SRK)[20]	4.87	2.90

The VLE data for the test systems were acquired from the large built-in database of Aspen Plus (v10) based on column pressure, thermodynamic model and number of data points (i.e. resolution) needed. Mathias[14] recommended a large number of data points for complex VLE diagrams; hence, 500 data points are generated for every mixture. The VLE diagrams of three of the mixtures listed in

Table 1 are illustrated in Figure 1b. In this figure, a distinction in the equilibrium characteristics of these mixtures is visible, which is important for understanding their influence on the overall column efficiency. The compositions of the more volatile component in condenser and reboiler streams (refer to Figure 1a) are maintained at 90% and 10%, respectively. This is based on the recommendation of Górak and Schoenmakers,[2] since extreme component purities in these streams may lead to errors in the VLE data analyses. It should be noted that the mixtures in Table 1 are arranged in the ascending order of α_{avg}, which is the average relative volatility of the light component relative to the heavy component. In the nomenclature of binary mixtures, the first compound is the light component, e.g., methanol is the more volatile component in the methanol-water mixture. Besides, the relative volatility (α) between the components is generally uniform over the entire column for hydrocarbon mixtures, whereas for aqueous systems, alcohol mixtures and other systems, α varies considerably over the column. In any case, the relative volatility is averaged over the column as

$$\alpha_{avg} = \sqrt{\alpha_T \alpha_B} \quad , \tag{4}$$

where α_T and α_B represent the relative volatilities of the streams leaving top and bottom of the column, respectively. Further, Lockett[1] and Kister[18] suggested to provide VLE data along with efficiency calculations. Thus, reduced VLE data (i.e. with 50 points) for each mixture are provided in Table S1 in the Supplementary Information. All 500 VLE data points for these mixtures are accessible in the RODARE repository.[23] In addition, Table 1 also mentions the minimum number of stages (N_{min}) needed in the column for each mixture based on the prescribed specifications of the condenser and reboiler streams. In fact, N_{min} also specifies the equilibrium number of stages in the column at total reflux, which can be calculated using the renowned Fenske's equation. However, Górak and Sorensen[5] reported that this equation is unreliable, when α varies noticeably over the column. Thus, these stages are obtained using the MT method applied in MATLAB (R2017b) as shown in Figure S1 in the Supplementary Information. In addition, Górak and Olujić[6] emphasized

the need of conservative approaches for estimating the column efficiency. Schultes[15] also agreed on the inclusion of safety margins in the column design, especially where information or experience pertaining to column design is incomplete or missing. Hence, the fractional number of equilibrium stages, as given in the Table 1, and actual number of trays rounded off to the next integer will be considered in eq 1 for conservative predictions of the column efficiencies.

2.2 Flow description on column trays

The description of the two-phase flow in a column is essential for its performance calculation. Basically, the information about the flow over one column tray would be sufficient, if the tray column is considered as a stack of trays that are geometrically and functionally similar.[3] Several studies in the literature claim that flow and mixing patterns of the individual phases have strong influence on the mass transfer characteristics of trays.[3] Plug flow is considered ideal for the tray performance.[12] Sahai and Emi[24] stated that mixing in the axial (i.e., flow-wise) direction is non-existent at plug flow, however, there may be mixing in the transverse direction (i.e., orthogonal to the main flow direction) to any extent. Shah et al.[24] supported this definition of plug flow only for complete mixing in the transverse direction. Any deviation from plug flow, referred to as non-ideal flow or flow maldistribution, is considered detrimental to the tray efficiency.[25] This holds for both liquid and vapor flow over the tray.[26] As observed in experimental studies reported in the literature,[3] liquid flow is represented by the residence time distribution (RTD) here, while presuming vapor plug flow through the trays. The RTD is a well-known concept in chemical engineering that is used for analyzing the flow behavior in continuous flow systems.[27] According to this concept, the fluid elements follow different routes in a system, and thus, require different times to leave it. The distribution of these times for the fluid elements leaving the system is represented by the RTD function ($f(t)$). For instance, the RTD functions for a plug flow reactor and an ideal

continuous stirred-tank reactor are $\delta(t-\tau)$ and $\tau^{-1}e^{-t/\tau}$, respectively. Here, τ is the mean residence time of the fluid elements defined as

$$\tau = \int_0^\infty t f(t) dt \quad . \tag{5}$$

An in-depth coverage of the RTD concept and the techniques for determining the RTD functions of systems can be found elsewhere.[28,29] Different models are used for describing the flow behavior (i.e., macromixing characteristics) in continuous flow systems, such as the axial dispersion model (ADM) and the tanks-in-series model (TISM), to name a few.[30] According to Levenspiel,[28] both these models are approximately equivalent to each other, but the physical basis of the TISM is not as clear as that of the ADM. The former describes the RTD in terms of integral number of ideal CSTRs only.[31] The analytical solution of the ADM for the open-open boundary condition provides the RTD function that is often preferred in the experiments[28] as

$$f(t) = \frac{1}{\sqrt{4\pi t \tau_h N_{TD}}} \cdot exp\left\{ -\frac{\left(1 - {}^{t}/_{\tau_h}\right)^2}{4tN_{TD}/\tau_h} \right\} \quad . \tag{6}$$

Here, τ_h is the hydraulic time that is based on bulk liquid velocity and flow path length (Z) of the tray. Further, N_{TD} is the dimensionless parameter referred to as tray dispersion number[25] that is defined as

$$N_{TD} = \frac{D_E \cdot \tau_h}{Z^2} \quad . \tag{7}$$

The reciprocal of the tray dispersion number is called Péclet number (Pe). In eq 7, D_E is the axial dispersion coefficient that characterizes liquid backmixing in a system.[25] Hence, higher dispersion number means higher liquid mixing in the axial direction on the tray, and vice-versa.[25] Based on these information, three different arbitrary RTD functions (Cases I to III) are prescribed to the liquid flow on the trays (by assuming dispersion numbers and hydraulic times in eq 6) as shown in Figure

2. This figure is presented with a limited time scale (i.e., up to 60 s) for better illustration of these functions. From Case I towards Case III, the dispersion number or the amount of axial liquid mixing on the tray is decreasing. The higher the axial liquid mixing on the tray, the higher the tray efficiency loss.[25] Therefore, the tray efficiency for constant point efficiency (E_{OV}) and stripping factor over the tray should be the lowest in Case I, intermediate in Case II, and the highest in Case III. This behavior will be inspected in detail in the upcoming sections.

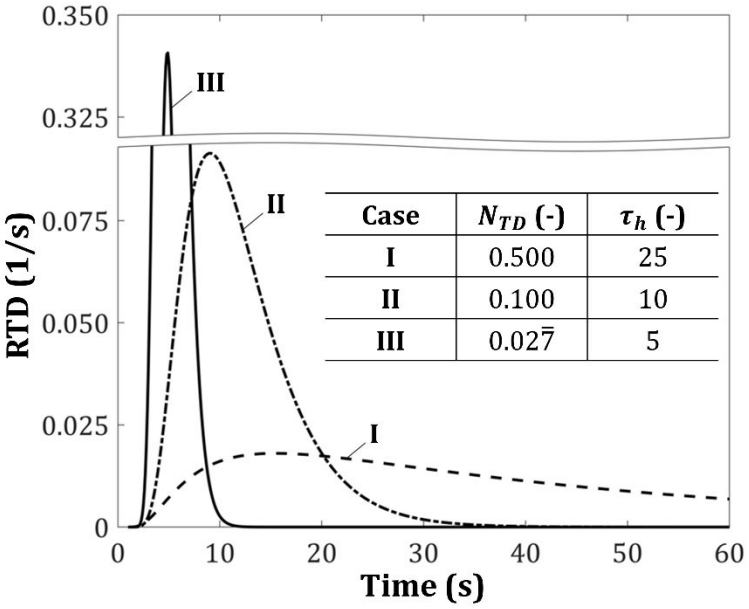


Figure 2. RTD functions and associated parameters of the three cases.

2.3 Tray-to-tray efficiency calculations

Kister et al.[32] proposed a sequence of steps for converting individual phase resistances into column efficiency via Lewis'[12] definition (eq 3) using information such as stripping factor, flow distribution, entrainment and weeping. Basically, this procedure assumes one tray as a representative for a section or the whole column, and estimates the section or column efficiency based on the selected tray conditions.[1] A similar approach is used here, as shown in Figure 3, except that tray-to-tray

efficiency calculations are preferred over eq 3. This allows to incorporate variations in hydraulic conditions, thermodynamic equilibrium, design characteristics and so forth, in the overall efficiency estimation.

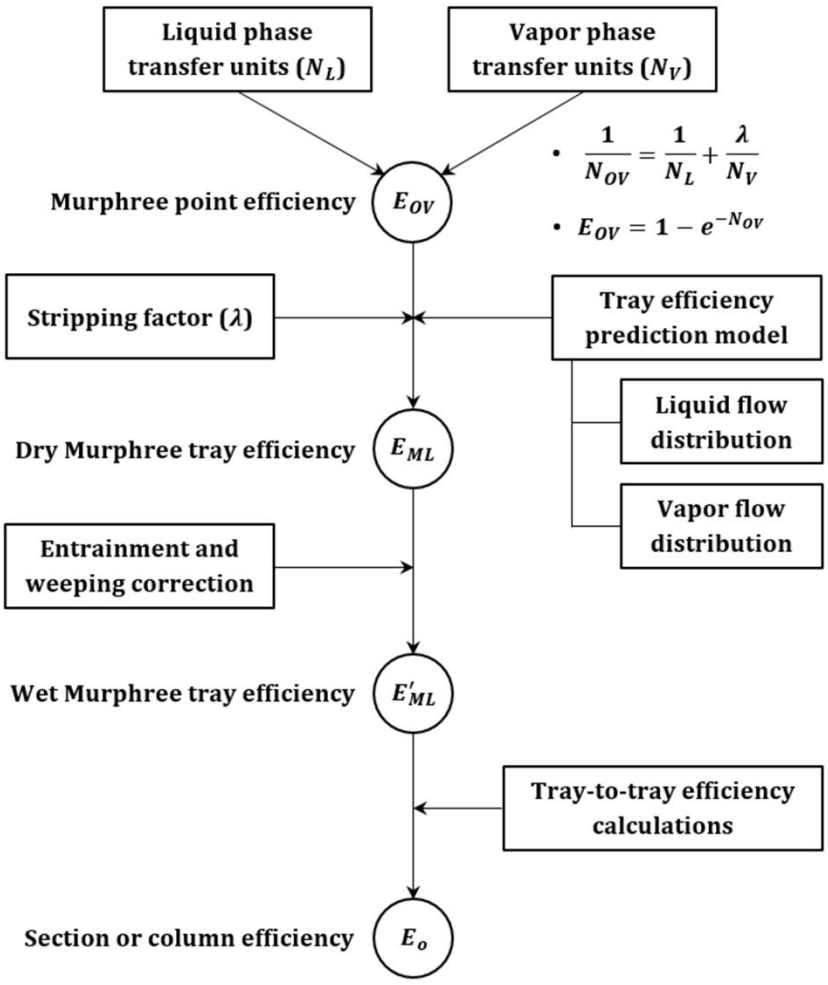


Figure 3. Sequence of steps for the section or column efficiency prediction.

Firstly, the vapor and liquid phase transfer units (referred to as N_V and N_L, respectively) are estimated based on the two-film resistance theory. The phase resistances are then added up to get the overall vapor phase transfer units (N_{OV}), from which the Murphree vapor-side point efficiency (E_{OV}) is estimated using an appropriate literature model.[1,32] Based on AIChE's bubble-tray design manual,[13] several studies have considered distillation to be a vapor-phase-controlled (i.e., negligible

liquid-phase resistance) operation.[33] However, experimental data in the literature[1,34-37] indicate that the liquid-phase resistance can also be significant.[33] To acknowledge these facts, the transfer units of the individual phases on the tray are considered as equal, i.e., $N_V = N_L$. This is applied to all trays in the column. No numerical values are prescribed to these units, since they require an individual description of mass-transfer coefficients, interfacial area, and residence times according to Lockett.[1] Instead, the point efficiency (E_{OV}) is considered to be constant on each tray in the column for the given equality. Two arbitrary cases of E_{OV} as 30% and 60% are considered here. This would further allow understanding their effect on the overall column efficiency. Then, a mathematical model is needed for converting the point efficiency into tray efficiency based on flow and mixing patterns of the individual phases and the VLE data.[32] Different tray efficiency prediction models are available in the literature, namely plug flow model,[12] pool models,[38-40] diffusional models,[41-43] non-uniform flow model,[44] RTD model,[45] and others.[25,26] The RTD model is selected here, because it accounts for all possible types of liquid flow behavior on a tray and thus, provides the most realistic estimation of the tray efficiency. According to this model, the Murphree vapor-phase and liquid-phase tray efficiencies are

$$E_{MV} = \frac{1 - \int_0^\infty e^{-\lambda E_{OV} t/\tau} \cdot f(t)dt}{\lambda \int_0^\infty e^{-\lambda E_{OV} t/\tau} \cdot f(t)dt} \quad \text{, and} \tag{8}$$

$$E_{ML} = \frac{1 - \int_0^\infty e^{-\lambda E_{OV} t/\tau} \cdot f(t)dt}{1 - \frac{1}{\lambda}\left\{1 - \int_0^\infty e^{-\lambda E_{OV} t/\tau} \cdot f(t)dt\right\}} \quad , \tag{9}$$

respectively. Foss[46] validated this model through oxygen-stripping studies on a rectangular sieve tray operated with oxygen-rich water and air. Detailed information regarding this model, especially its mathematical formulation, associated assumptions and experimental validation, can be found elsewhere.[3,25,45,46] Three RTD functions (Cases I to III) representing the liquid flow on the column trays are already defined (see Section 2.2) for the model application. The mean residence time for

each case can be calculated using eq 5. In addition, plug flow of vapor through the trays and perfect mixing in the disengagement zones between them are assumed in this model. Recently, new tray concepts[47-50] have demonstrated reasonably uniform vapor distribution, and hence, the standard efficiency prediction models are directly applicable to those trays. Besides, based on the assumption of linear VLE relationship (for an expected composition range over a tray) and the total reflux operation, λ for a tray reduces to the slope (m) of the VLE line.

As per authors' knowledge, the only known approach for calculating m can be found in AIChE's design manual.[13] That approach was proposed for VLE data with large curvature only, and by assuming that liquid on the tray is perfectly mixed. This implies that the tray and point efficiencies are the same for the tray (e.g., $E_{MV} = E_{OV}$),[3] while E_{MV} is usually greater than E_{OV} due to imperfect (or partial) liquid mixing on the tray.[1] Hence, a more general approach that is devoid of the limitations stated above is explained in Figure 4. This figure is provided for illustration only and does not depict any particular case of column simulation. For better understanding of the explanations below, the top-to-bottom approach is applied for labelling the trays as well as for the efficiency calculations.[5] According to Lockett,[1] E_{MV} and E_{ML} should be preferred when moving up and down in the column, respectively. In this study, eq 9 and the common definition of E_{ML}, i.e.,

$$E_{ML} = \frac{x_n - x_{n-1}}{x_n^* - x_{n-1}} \quad , \tag{10}$$

for the n^{th} tray is used. In eq 10, x_{n-1} and x_n are the average compositions of the liquid stream entering and leaving the n^{th} tray, respectively, and x_n^* is the liquid composition that is in equilibrium with the composition of vapor exiting that tray. According to eqs 9 and 10, an accurate determination of λ (or m) is essential for correct values of E_{ML} and x_n.

For any given x_{n-1} (i.e., the composition of the reflux liquid at column top here), the corresponding x_n^* can be obtained using the MT method as shown in Figure 4a. The nomenclature of each line used in Figure 4 is also provided there. In the new approach, m is initially assumed for the tray, and the

resulting E_{ML} and x_n are calculated using eqs 9 and 10, respectively. These parameters are then iterated collectively and progressively until the variations in each of their successive numerical values are less than 10^{-4}. For doing so, it is crucial to identify the range of the VLE data that needs to be considered for the slope calculation specific to a tray. Such range depends on the transfer units and the molar flow rates of the two phases as suggested in AIChE's manual.[13] For this purpose, the supporting lines are drawn with the slope $\beta = {(-N_L \cdot L)}/{(N_V \cdot V)}$ from x_n^* and x_{n-1} on the diagonal line. Since $N_L = N_V$ and $L = V$, the slope of these lines is 135° as shown in in Figure 4b. In the same figure, the supporting lines intersect the VLE curve at points i^* and j, respectively. Between i^* and j , the VLE curve is fitted (in the least-squares sense) with a straight line using the 'polyfit' function in MATLAB (refer to Figure 4c). The slope of the fitted line is the initial estimate called m^* there. As given in Remark 1 in Figure 4, m^* is then supplied to eq 9 for calculating E_{ML}. From this E_{ML}, the first estimate of x_n, referred to as x_n^1, is obtained using eq 10 (see Figure 4d). Since x_{n-1} is fixed for the tray, the location of point j on the VLE curve remains unchanged throughout in Figure 4. Now, the supporting line with the slope β is drawn from point x_n^1 on the diagonal line intersecting the VLE curve at i^1 as shown in Figure 4d. Then, the VLE curve between i^1 and j is fitted with a straight line, as explained earlier, to obtain the new estimate of m (referred to as m^1 in Figure 4e). According to Remark 2 in Figure 4, the new value of x_n (called x_n^2) is estimated as shown in Figure 4f. The procedure discussed so far is repeated (e.g., k times in Figure 4g) until the difference in the consecutive numerical values of each m, E_{ML} and x_n is below 10^{-4}. Not more than 10 iterations were required to satisfy the prescribed criteria. Eventually, the correct values of m (= m^k, not shown here), E_{ML}, i^k, and x_n (= x_n^k) are obtained as shown in Figure 4g. Here, point i^k represents liquid and vapor compositions at the interface, where the vapor enters the tray. Similarly, point j represents these compositions at the interface, where the vapor leaves the tray.[13] Furthermore, it is assumed that there is no entrainment and weeping, which leads to $E_{ML} = E'_{ML}$ in Figure 3. So, the estimated composition of the liquid stream exiting the n^{th} tray becomes the inlet composition for the next tray.

This was considered in the graphical study of Mathias,[14] which can happen because of perfect liquid mixing in the downcomer. This entire procedure involving eqs 9 and 10, and Figures 3 and 4 is repeated for the next tray and so forth, until the actual tray step reaches the composition of the liquid leaving the column at the bottom, which is 0.1. This way, the efficiency of each tray, and hence, the actual number of trays in the column are calculated. The readers are referred to Lockett,[1] Kister et al.[32] and Foss[46] for the assumptions (not given here) involved in the mentioned steps in Figure 3.

An alternate approach to the line fitting method proposed above is the averaging of the slope of the VLE curve over the required range. Such an approach can also be used for the slope estimation in Figures 4c, 4e and others. For instance, the VLE curve between points i^k and j in Figure 4g is firstly fitted with a second degree univariate polynomial (i.e., $y(x) = ax^2 + bx + c$) using the 'polyfit' function in MATLAB. Here, a,b and c are the coefficients of this polynomial with $a \neq 0$. Thus, calculating the derivative of this quadratic function (i.e., $y'(x) = 2ax + b$) at each abscissa point between points i^k and j and averaging the resulting y' values provides m for the tray. Both approaches are equivalent and produce identical values of m for each column tray. This is exemplarily shown for the binary systems water-acetic acid, benzene-toluene, and methanol-water in Table S2 in the Supplementary Information.

Space left for Figure 4

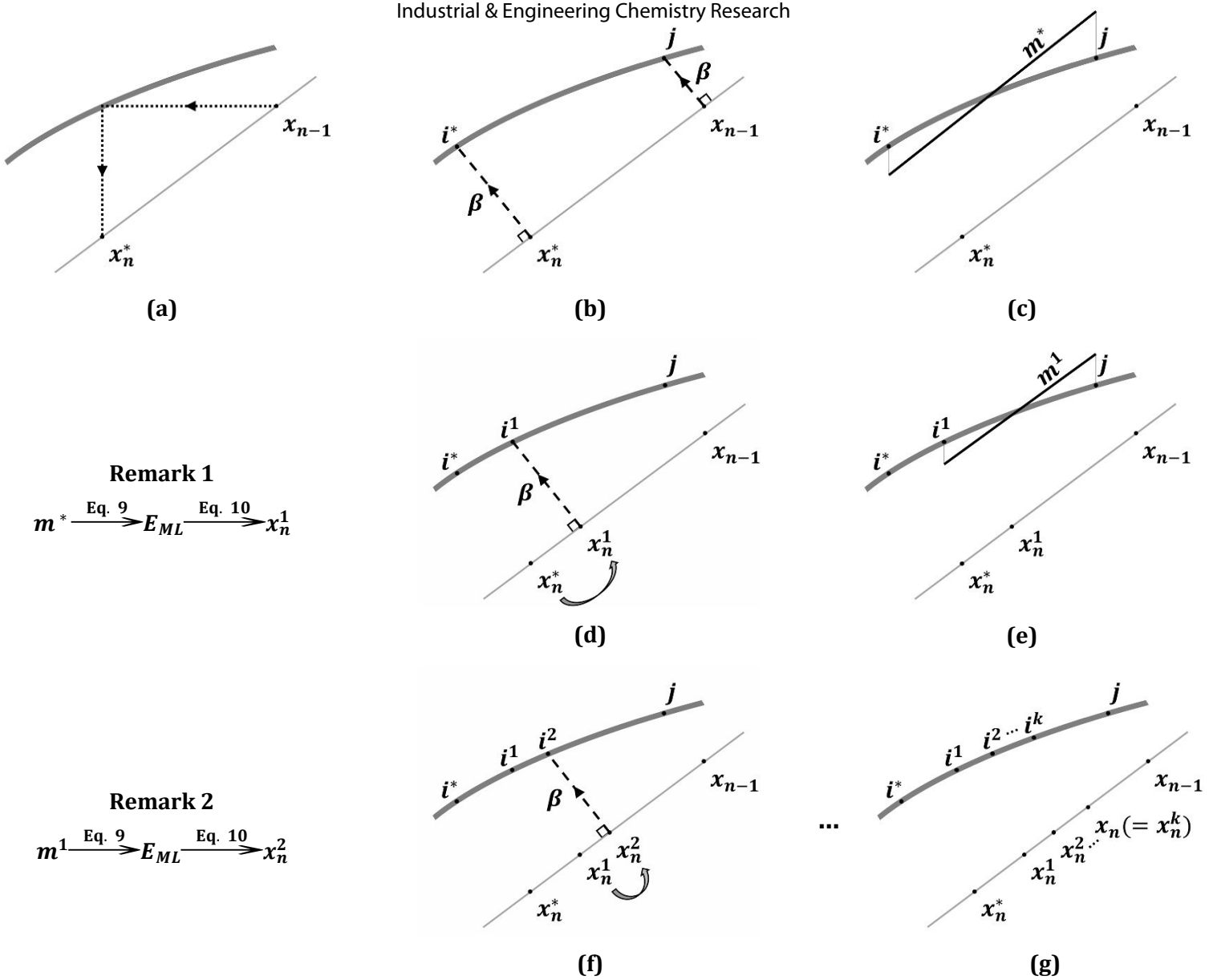
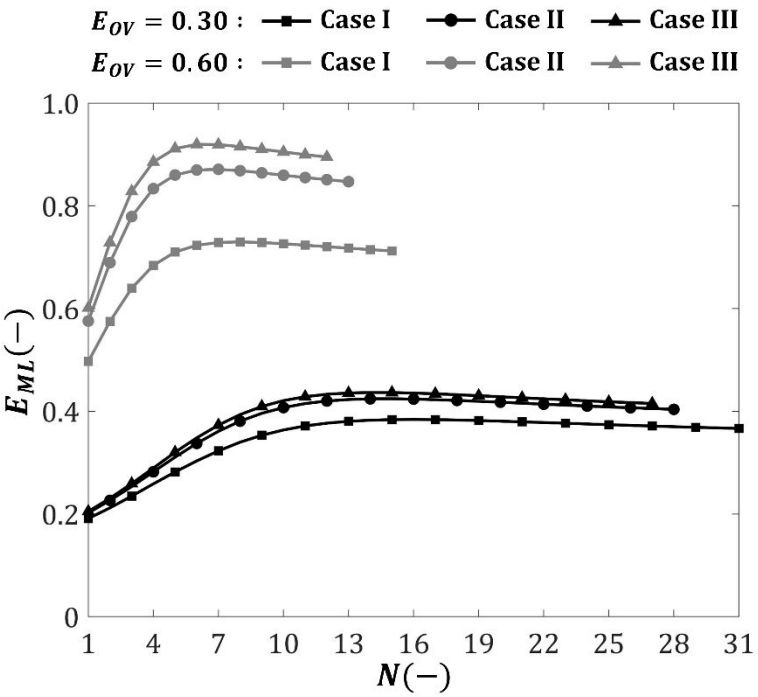


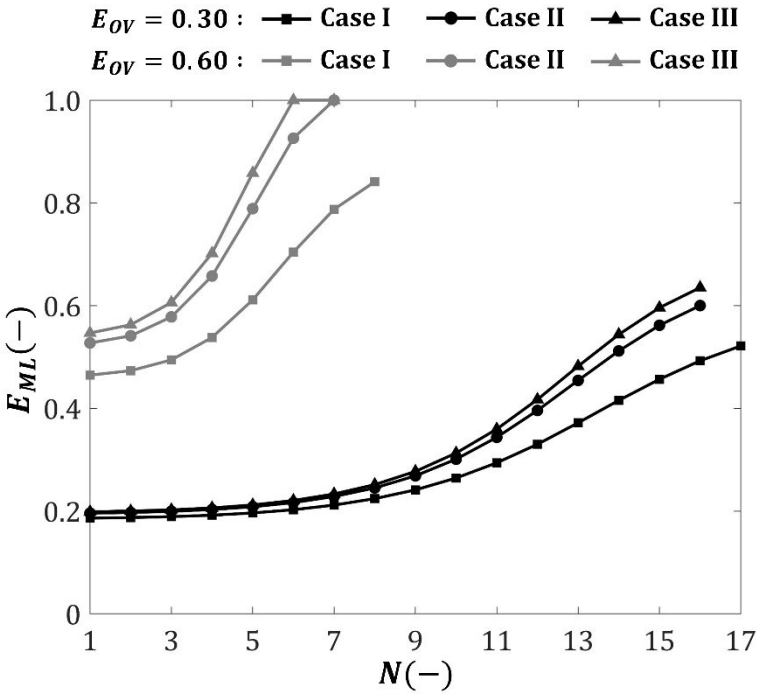
Figure 4. Graphical illustration for estimating the slope of the VLE line (not drawn to scale, figure details and explanations are provided in the text).

2.4 Tray and column efficiency predictions

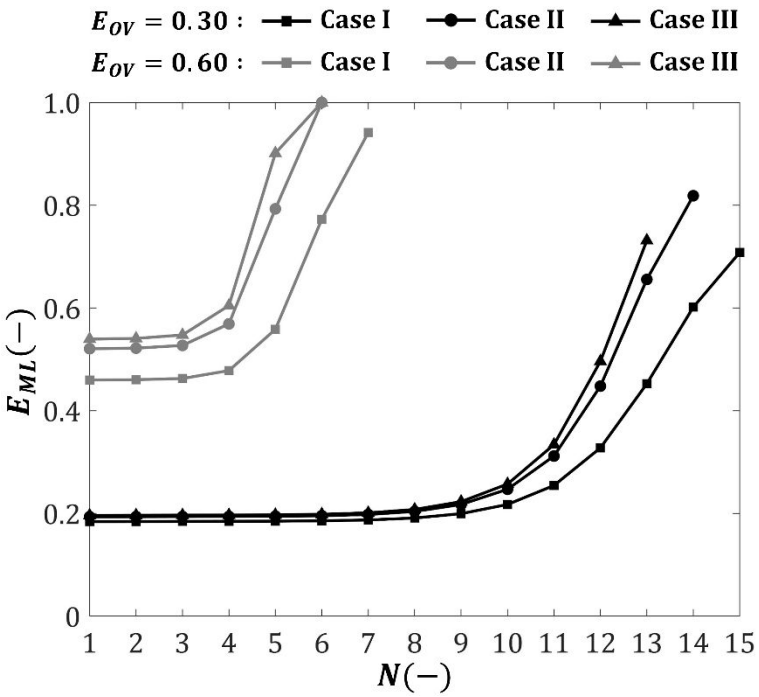
Based on the procedure explained in Section 2.3, the actual number of trays in the column and their efficiencies are calculated for each mixture. The tray efficiency predictions for the three mixtures, whose VLE profiles are shown in Figure 1a, are presented in Figure 5. The predictions for the remaining mixtures listed in Table 1 are provided in Figure S2 in the Supplementary Information. For any given liquid dispersion and point efficiency on the tray, the variation in the tray efficiency (according to eq 9) is caused by the variation of m over the trays in the column (refer to Table S2 in the Supplementary Information). In fact, the variation in m is because of that in the VLE at different temperatures at constant total pressure (see Table S1 in the Supplementary Information). Accordingly, the tray efficiencies vary over the column height for the mixtures for prescribed flow profiles and point efficiencies on the trays. Referring to the x-y plots and efficiency estimates pertaining to the hydrocarbon mixtures in Figures 5, S1 and S2, the difference between the upper and lower limits of m, and hence, the tray efficiency increases with increasing α_{avg}. Hence, using the proposed approach, any variation in the VLE data of a binary mixture can be considered in the column efficiency prediction, since the actual number of trays is known after the tray efficiency calculations. Postulating that m along with flow profiles and point efficiencies remain constant over the trays, then each tray in the column would perform with the same efficiency. This simplification is followed in AIChE's manual using eq 3 for column efficiency predictions,[13] which is currently the most applied method in the literature. The refined procedure proposed here is clearly superior in this regard.



(a) Water-acetic acid



(b) Benzene-toluene



(c) Methanol-water

Figure 5. Tray efficiency predictions based on VLE data, flow profiles and point efficiencies for selected mixtures. (cases of liquid backmixing: I – severe, II – intermediate, and III – low)

Space left for Figure 6

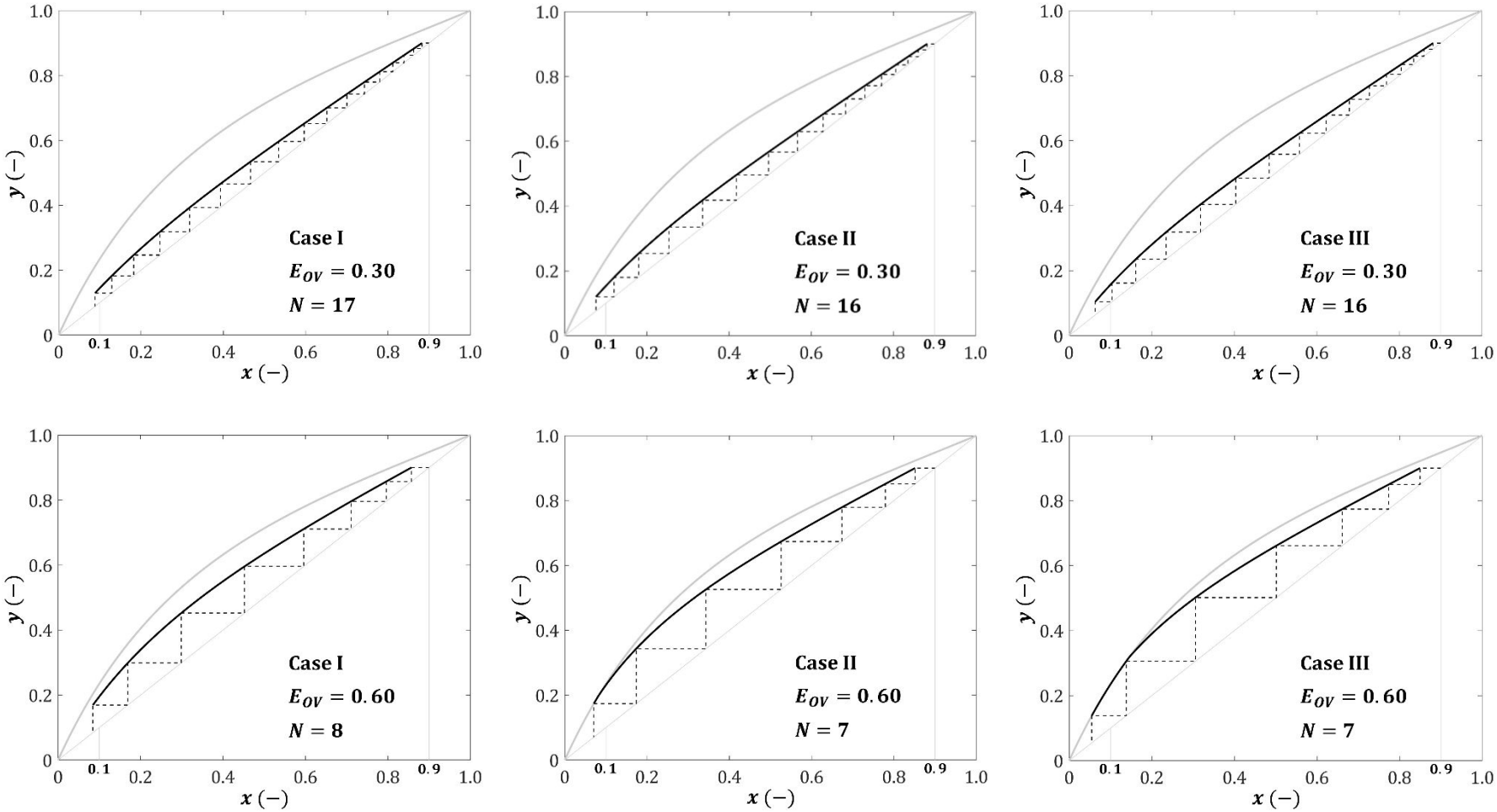


Figure 6. Actual number of trays obtained through efficiency evaluations on the *x*-*y* charts for the benzene-toluene mixture. (cases of liquid backmixing: I – severe, II – intermediate, and III – low)

For a constant point efficiency on each tray, the tray efficiency is expectably the lowest in Case I, intermediate in Case II, and the highest in Case III (see Figure 5 earlier and Figure S2 in the Supplementary Information). This happens because the amount of axial liquid mixing associated with each RTD function decreases from Case I to Case III (see Section 2.2). Further, the tray efficiency increases with increasing point efficiencies for given RTD functions and estimated slopes on each tray. Hence, the number of trays actually needed in the column for achieving the targeted separation task is the highest in Case I, intermediate in Case II, and the lowest in Case III at constant point efficiency on each tray. In this scenario, the corresponding number of trays in each case reduces upon the rise in the point efficiency. Moreover, the estimated values of m are fairly high on the lower trays in the column for some mixtures. This can be visualized in the x-y charts shown in Figure S1 in the Supplementary Information. When the higher values of m combine with low axial liquid mixing and high point efficiencies, then the corresponding tray efficiencies becomes greater than unity (not shown here). It is possible for the Murphree tray efficiency to exceed unity especially for large columns and systems of high relative volatilities.[32,51] In that case, the resulting tray step (as illustrated in Figure 4) would actually transcend the VLE curve. Thus, the maximum tray efficiency is limited to unity here. For example, the efficiencies of the Trays 6 and 7 in the column processing the benzene-toluene mixture in Case III at E_{OV} = 0.60 are higher than 100%. Hence, the efficiencies of these trays are restricted to their prescribed limit as shown in Figure 5b. This restriction is also applied to other mixtures. These findings about the tray efficiencies and the resulting number of trays can also be visualized in the x-y charts shown for the benzene-toluene mixture in Figure 6 (x-y charts for the remaining two mixtures considered in Figures 1b and 5 are provided in Figure S3 in the Supplementary Information). The dashed line steps convey the predicted tray efficiencies based on the estimated slopes, considered dispersion numbers and point efficiencies. The black continuous curve depicts the locus of the compositions of liquid and vapor streams exiting the trays for each given condition. This curve is referred to as pseudo-equilibrium curve in the literature.[52] It can be deduced that the column requires

higher number of (actual) trays, when the pseudo-equilibrium curve shifts towards the diagonal line. On the other hand, lower number of trays are needed in the column, when the pseudo-equilibrium curve shifts towards the VLE curve. Besides, for mixtures with high α_{avg}, the pseudo-equilibrium curve overlaps with a certain range of the VLE curve in the lower part of the column. This can be observed in the Cases II and III at E_{OV} = 0.60 in Figures 6e, 6f and S3 in the Supplementary Information. This is because the maximum tray efficiency is limited to unity in this work.

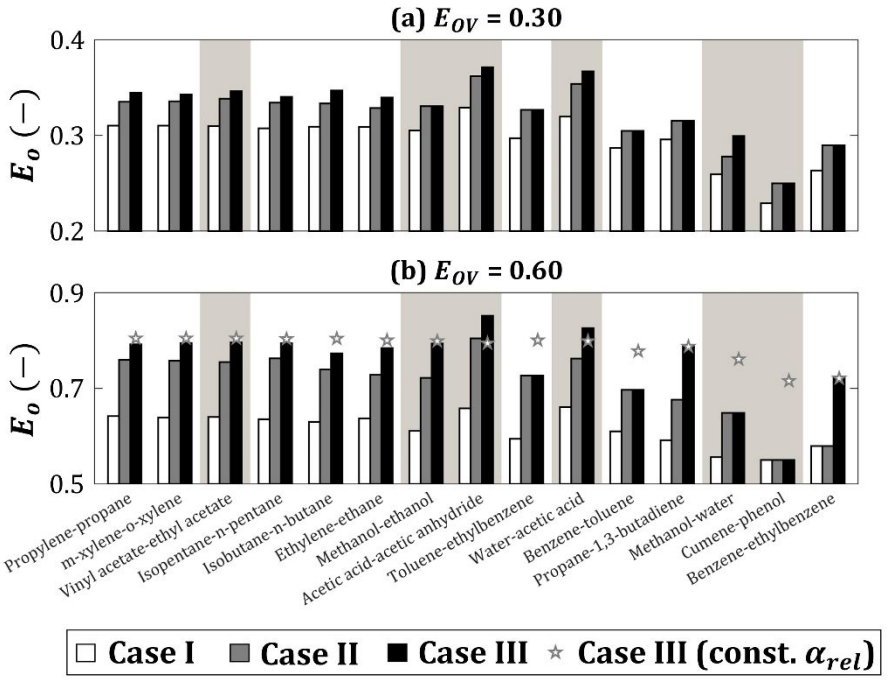


Figure 7. Overall column efficiency predictions for the considered binary mixtures. (cases of liquid backmixing: I – severe, II – intermediate, and III – low)

Figure 7 summarizes the determined overall column efficiency for each mixture depending on given RTD functions, point efficiencies and estimated slopes. Here, the mixtures are arranged on the x-axis in an increasing order of their α_{avg}. In this figure, the predictions with white background correspond to hydrocarbon mixtures, whereas the remaining mixtures are displayed with grey background. As stated

earlier, the column efficiencies are determined here based on fractional number of equilibrium stages, and actual number of trays rounded off to the next integer using eq 1. For any particular point efficiency on the trays, the column efficiency is the lowest in Case I, intermediate in Case II, and the highest in Case III for each mixture. This is because the number of trays needed in the column for the targeted separation task reduces from Case I to Case III owing to the reduction in axial liquid mixing on them (see Figures 5 and S2 in the Supplementary Information). Further, for any particular RTD function, the column efficiency increases with the point efficiency for each mixture. Besides, for some mixtures (especially with high relative volatilities), the column efficiency remains constant in Figure 7 irrespective of the liquid dispersion on the trays at a given point efficiency. For example, the overall efficiencies of the column processing benzene-toluene mixture in Cases II and III are the same. This is because the fractional numbers of actual trays for this mixture are 15.5 and 15.1 at E_{OV} = 0.30, and 6.7 and 6.5 at E_{OV} = 0.60, respectively. Rounding off these numbers to the next integer conceals the effect of the flow profiles on the column efficiency in case of mixtures with high α_{avg}. Hence, the fractional number of actual trays for each mixture is provided in Table S3 in the Supplementary Information for the given cases. Furthermore, the trend of efficiency predictions for the given mixtures can be examined via predictions corresponding to the hypothetical mixtures. Therefore, the column efficiency predictions for 15 hypothetical mixtures with constant α over the trays (with the numerical values same as α_{avg} given for the mixtures in Table 1) are presented only for Case III at E_{OV} = 0.60 in Figure 7. For hypothetical mixtures, the simulation starts with their VLE data, which is obtained using

$$y = \frac{\alpha \cdot x}{1 + (\alpha - 1) \cdot x} \quad . \tag{11}$$

Following the procedure discussed in the Sections 2.2 and 2.3, the column efficiencies are estimated by computing N_{min} and N without rounding off. The column efficiencies of these mixtures are nearly uniform until $\alpha = 2$, that approximately corresponds to the toluene-ethylbenzene mixture in Figure 7. For $\alpha \geq 2$, the column efficiencies of the hypothetical mixtures decline as shown in this figure. If the

fractional values of N are used in eq 1 for the hydrocarbon mixtures, then their column efficiencies are nearly identical to those of the corresponding hypothetical mixtures (not shown here). Of course, this holds for the same dispersion number and point efficiency on the column trays for those mixtures. This happens because α is approximately uniform in case of hydrocarbon mixtures. These observations also hold for other mixtures with low α_{avg}, such as vinyl-acetate-ethyl acetate and methanol-ethanol, since the variation in α is insignificant for those mixtures. However, α varies significantly for other mixtures with higher α_{avg} (such as those given in Figure 1b), where the column efficiencies do not follow the trend of those of the corresponding hypothetical mixtures upon considering fractional values of N in eq 1. For these mixtures, when α values are lower on the top tray than those on the bottom tray, then the column efficiency is also lower than that of the corresponding hypothetical mixture, and vice-versa. For example, the mean values of α for topmost and bottommost trays for acetic acid-acetic anhydride, methanol-water, and cumene-phenol mixtures are approximately 2.8 and 1.0, 2.1 and 5.0, and 2.4 and 8.2, respectively. Thus, with respect to the estimations pertaining to the corresponding hypothetical mixtures in Figure 7, the column efficiency is higher for acetic acid-acetic anhydride mixture, and lower for methanol-water and cumene-phenol mixtures. Further, when the difference between the mean α values on topmost and bottommost trays is high, then the difference between the column efficiency and that of the corresponding hypothetical mixture is also high, and vice-versa. This can be seen for the estimations related to methanol-water and cumene-phenol mixtures in Figure 7. Moreover, binary mixtures with high relative volatilities are easy to separate via distillation, and hence require less number of trays in the column.[5] However, this is only possible when the column trays operate with low liquid backmixing and high point efficiency. Otherwise, higher number of trays are needed for the separation target, thereby deteriorating the overall column efficiency.

3. Case study II

The application of the proposed procedure for efficiency estimation of an industrial column is attempted in this section. More than a decade ago, Taylor[16] reported the scarcity of the real column data of sufficient quality in the accessible literature that could be used for performance evaluation, which still holds for today. As per authors' knowledge, the only performance data of an operational column that can be used in this work is available in AIChE's reports cited here.[13,41] The details of the available data followed by efficiency calculations are discussed in the following section.

3.1 Background information

The aforestated reports provide performance test data of a column operated by Eastman Kodak (New York). A 1.66 m diameter column, containing 60 single-pass bubble-cap trays (labelled from the bottom), was operated in the total reflux mode in three different test runs. In the calculation sheet of AIChE's manual,[13] the first test run is considered for predicting the column efficiency using eq 3. Hence, the information only pertaining to the first test run is considered here. The mixture of methylene dichloride (CH_2Cl_2) and ethylene dichloride ($C_2H_4Cl_2$) was processed in the column at an average total pressure of 2.34 bar. For this system, 10 VLE (i.e., temperature-mole fraction) data points were provided considering ideal phases of liquid and vapor. Liquid samples were withdrawn from different trays under steady-state conditions. It was found that the Trays 1 to 27 contained almost pure ethylene dichloride, whereas the Trays 35 to 60 had nearly pure methylene dichloride. Technically, these trays were inactive as far as thermal separation is concerned. The data for the inlet liquid composition were given for the Trays 34, 32 and 28 as 99.40%, 95.94% and 18.20%, respectively. According to the recommendation of Górak and Schoenmakers,[2] extreme component purities are avoided in the present work, and hence, the section involving the Trays 32 to 29 (4 trays) is considered. Further, the tray and point efficiencies were determined experimentally for Tray 32. For this tray, the numerical values given for N_L, N_V, Pe, E_{OV} and E_{MV} are 1.55, 13.0, 27.8, 77.2% and 84.5%, respectively. Further details

about the column and tray design, plant test data and procedure, and determination of the given parameters can be found in the recommended literature.

Based on the earlier-mentioned decision tree,[20] the UNIQUAC model is selected to obtain more reliable and high resolution VLE data for the given system. Applying this model and the provided total pressure in Aspen Plus (v10), 500 VLE data points are generated that can be acquired from the RODARE repository.[23] The reduced VLE data (i.e. with 50 points) for this mixture are also provided in Table S4 in the Supplementary Information. According to eq 4, the average relative volatility over the selected column section is 3.89. Then, using the MT method, N_{min} is obtained as 3.63 as shown in Figure S4 in the Supplementary Information. Substituting the fractional value of N_{min} and the actual number of trays (= 4) in eq 1 determines the actual section efficiency that is 90.75%. This efficiency is used here for evaluating the prediction from the proposed procedure as well as that from eq 3.

3.2 Tray and column efficiency predictions

Following the sequence of steps illustrated in Figure 3, the trays are stepped from bottom to top as originally labelled in the column. Similar to Case study I (see Section 2.3), it is assumed that the given parameters such as phase transfer units (N_L and N_V), point efficiency (E_{OV}), and Péclet number (Pe) for the liquid flow remain same on each tray. Then, the AIChE model is recommended in the mentioned reports for predicting the tray efficiencies based on these given parameters. In the literature,[3,41] this model is formulated through mass balancing on the two-phase dispersion on a tray as

$$\frac{E_{MV}}{E_{OV}} = \frac{1 - exp\{-(\eta + Pe)\}}{(\eta + Pe)\left(1 + \frac{\eta + Pe}{\eta}\right)} + \frac{exp(\eta) - 1}{\eta\left(1 + \frac{\eta}{\eta + Pe}\right)} \quad \text{, where} \tag{13}$$

$$\eta = \frac{Pe}{2}\left(\sqrt{1 + \frac{4\lambda E_{OV}}{Pe}} - 1\right) \quad . \tag{14}$$

This model assumes a linear VLE relationship and a constant point efficiency for the tray. Although not explicitly mentioned, plug flow of vapor through the tray with perfect mixing in the disengagement space between the consecutive trays is considered in the model formulation. This model considers liquid backmixing on the tray through Pe, which is referred to as 'simple backmixing model' by Porter et al.[42] Again, λ reduces to m in the above equation because of the total reflux operation and the linear VLE assumption. Similar to the procedure explained in Section 2.3, m and E_{MV} are estimated using

$$E_{MV} = \frac{y_n - y_{n-1}}{y_n^* - y_{n-1}} \quad , \tag{15}$$

and the AIChE model for the lowest tray in the section (i.e., Tray 29 with outlet liquid composition as 18.2%). The reader should note, however, that the labeling convention used for the trays in the column is from bottom to top in eq 15, whereas the top-to-bottom approach is considered in eq 10. Further, an operating line is a relationship between the compositions of vapor and liquid entering and leaving the trays in a section, respectively, that is based on the assumption of constant molar overflow.[5] Therefore, for Tray 29, the outlet liquid composition becomes the inlet vapor composition, because the operating line for this section is the diagonal line. Besides, no correction for the tray efficiency regarding entrainment and weeping was provided in the reports, and hence, it is neglected for all trays here. Eventually, the entire procedure for determining the tray efficiencies in the section is repeated until the stepping procedure reaches to the liquid composition exiting Tray 33 as shown in Figure 8. Moreover, the maximum limit for the tray efficiency is again prescribed as 100% here. The estimated value of m decreases from bottom to top in the column, which gets reflected in the tray efficiency predictions in this figure. The occurrence of low axial liquid mixing, high point efficiency and high values of m on the trays lead to higher tray efficiencies. Therefore, the pseudo-equilibrium curve in Figure 8 (displayed as the black continuous curve) lies in the immediate vicinity of the actual VLE curve (shown as the gray continuous curve). Further, the estimated values of m and E_{MV} for Tray 32 are 0.28 and 85.6%, respectively. This observation validates the AIChE model, since the predicted tray efficiency agrees

well to that obtained in the performance test run.[13] Further, these estimations recommend 4 trays in the section for the given composition specifications. Therefore, the proposed procedure estimates the section efficiency that is same as the actual. This agreement also justifies the prescribed limitation of the maximum tray efficiency as unity in this procedure. In fact, the typical values for the tray efficiency range between 50% and 70% according to Cheremisinoff.[53] As stated earlier, the information pertaining to Tray 32 were used for predicting the section efficiency in AIChE's manual. Based on those information, the section efficiency according to eq 3 is 75.4%, which is clearly an underestimation. If the manual's approach is explored for the remaining trays, i.e., for Trays 29, 30, and 31, the estimated section efficiencies are 100%, 100% and 83.8%, respectively. Different predictions for the section efficiency are obtained because of the different numerical values of m, and hence, E_{MV} on each tray. The only prediction involving eq 3 that is close to the actual section efficiency is based on the information of Tray 31, which could be fortuitous. Any rule for selecting a particular tray whose conditions are susceptible for an accurate section or column efficiency prediction is unknown and there may not be any such rule in reality. Besides, a deterministic approach is needed for meaningful estimation of the column and section efficiencies that are based on flow profiles and VLE data. Such requirement favors the applicability of the proposed procedure over that employed in AIChE's manual. Simple empirical models (e.g., O'Connell's correlation) are inapplicable for efficiency comparison here, because they require feed liquid viscosity as an input (see eq 2). Indeed, more performance data from industrial columns are needed in the literature for further analyzing the capabilities of the proposed procedure.

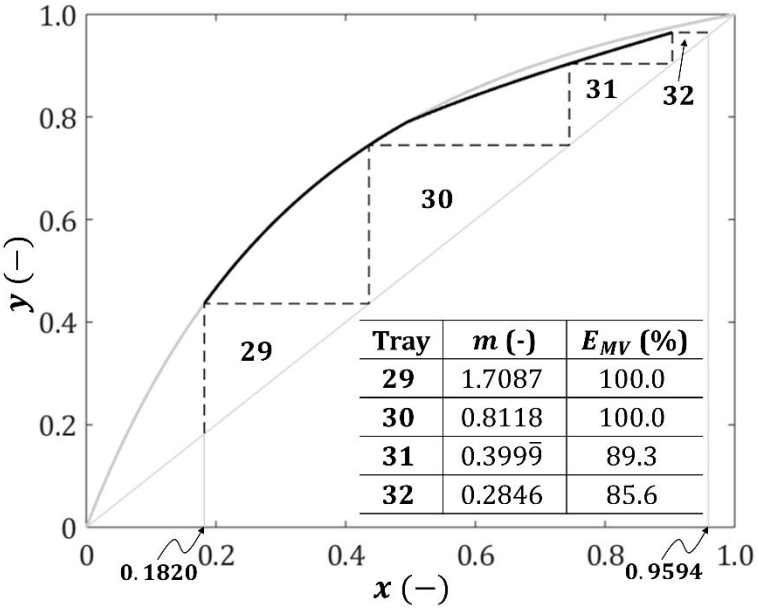


Figure 8. Slope and tray efficiency estimations along with the pseudo-equilibrium curve for the column processing methylene dichloride-ethylene dichloride mixture.

4. Conclusion and future work

A new systematic approach for estimating the column and section efficiencies based on flow profiles on the trays and VLE characteristics of binary mixtures has been proposed in this work. Such an approach would allow a priori estimation of the column performance in the tray and column design phase. This could be advantageous for the industry, as sometimes the potential areas for improving tray and column performances become known after the design phase leading to considerable losses in terms of cost and energy. A key feature of the proposed approach is the approximation of the slope of the VLE curve and the Murphree tray efficiency using an iterative technique. The capabilities of the new approach are demonstrated in two case studies, where the impact of point efficiencies, flow distributions and VLE data on the column efficiencies are presented. These information have not been considered exclusively for each tray by the existing approaches pertaining to column efficiency

estimation. A detailed analysis of the case studies confirms the superiority of the new approach over the most applied method in the literature.

In the future, an advanced tray efficiency prediction model[25] capable of considering vapor maldistribution on the trays could be considered in the proposed approach. Such an inclusion is expected to refine the predictive capabilities of this approach. Additionally, if pressure variations over the column height are known, then their impact on the tray column performance can also be investigated using the new approach.

Supporting Information Available

VLE data for binary mixtures obtained from various thermodynamic models at representative column pressures in Case Study I; Estimation of slope of the VLE curve in Case Study I (approach 1: line fitting, approach 2: slope averaging); Fractional number of actual trays for each mixture in Case Study I; VLE data of methylene dichloride-ethylene dichloride mixture in Case Study II; Minimum number of stages for each mixture (in the ascending order of α_{rel}) using the McCabe-Thiele method; Tray efficiency predictions for binary mixtures based on prescribed flow profiles and point efficiencies. (cases of liquid backmixing: I – severe, II – intermediate, and III – low); Actual number of trays obtained through efficiency evaluations on the x-y charts for (a) water-acetic acid, and (b) methanol-water mixtures. (cases of liquid backmixing: I – severe, II – intermediate, and III – low); Minimum number of stages in Case study II (methylene dichloride-ethylene dichloride, P = 2.34 bara, N_{min} = 3.63) based on McCabe-Thiele method.

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Notes

The authors declare no competing financial interest.

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Nomenclature

D_E	Eddy diffusion coefficient (m^2/s)
E_{ML}	Murphree liquid-phase tray efficiency (-)

E'_{ML}	Murphree liquid-phase tray efficiency corrected for entrainment and weeping (-)
E_{MV}	Murphree vapor-phase tray efficiency (-)
E_{OV}	Murphree vapor-phase point efficiency (-)
E_o	Section or overall column efficiency (-)
$f(t)$	Residence time distribution function (s^{-1})
i, j	Intersection of supporting lines with the VLE curve (-)
k	Iteration index in the slope calculation (-)
L	Liquid flow rate (mol/s)
m	Slope of the VLE line (-)
N	Actual number of trays (-)
N_{eq}	Number of equilibrium stages (-)
N_L	Number of binary liquid-phase transfer units (-)
N_{min}	Minimum number of trays (-)
N_{OV}	Number of overall binary vapor-phase transfer units (-)
N_{TD}	Tray dispersion number (-)
N_V	Number of binary vapor-phase transfer units (-)
P	Total pressure (bar)
Pe	Péclet number (-)
t	Time (s)
V	Vapor or gas flow rate (mol/s)

x	Composition (mole fraction) of the volatile component in the liquid phase (-)
x_n	Composition of the liquid stream exiting the n^{th} tray (-)
x_n^*	Liquid composition that is in equilibrium with the vapor exiting the n^{th} tray (-)
x_{n-1}	Composition of the liquid stream entering the n^{th} tray (-)
y_n	Composition of the vapor stream exiting the n^{th} tray (-)
y_n^*	Vapor composition that is in equilibrium with the liquid exiting the n^{th} tray (-)
y_{n-1}	Composition of the vapor stream entering the n^{th} tray (-)
y	Composition (mole fraction) of the volatile component in the vapor phase (-)
Z	Flow path length (m)

Greek Letters

α	Relative volatility (-)
β	Slope of the supporting line in Figure 4 (-)
δ	Dirac delta function (s^{-1})
λ	Stripping factor $\left(=mV/L\right)$ (-)
μ_L	Average liquid viscosity of the feed (mPa-s)
τ	Mean residence time of liquid on a tray (s)
τ_h	Hydraulic or space time (s)

Subscripts

avg	Average
B	Bottom stream
L	Liquid
n	n^{th} tray
T	Top stream
V	Vapor or gas

Abbreviations

ADM	Axial dispersion model
$AIChE$	American Institute of Chemical Engineers
MT	McCabe-Thiele
RTD	Residence time distribution
VLE	Vapor-liquid equilibrium

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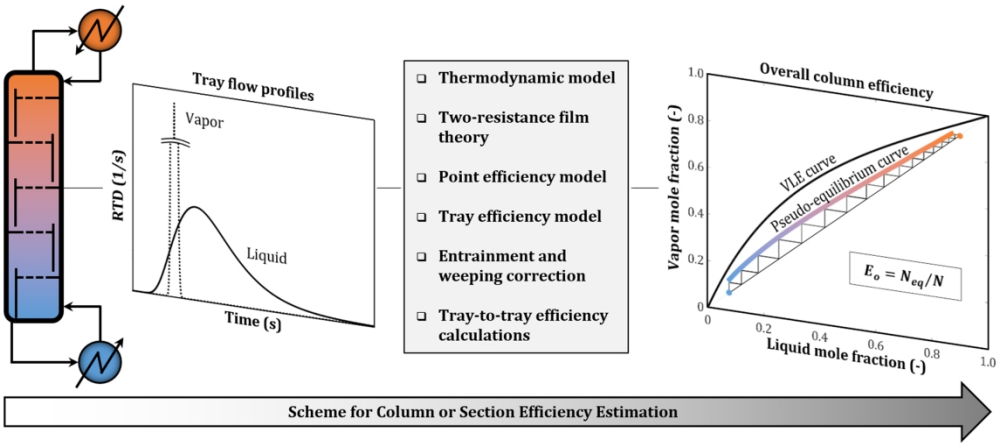

TOC graphic

338x150mm (300 x 300 DPI)