



Short communication

## Moving boundary in non-equilibrium simple batch distillation in non-ideal systems

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## ABSTRACT

This work is concerned with the computational aspects of the dynamic behavior of a simple distillation process using the irreversible model. The composition trajectories in residue curve map diagrams were calculated for a methanol/isopropanol/water mixture. The composition paths calculated by the irreversible model were compared to published experimental results for this mixture. The simulation results showed that residue curves, including the simple distillation boundaries, were sensitive to the irreversible model applied. Furthermore, since simple distillation boundaries and residue curves had been constructed using the same model equilibrium and irreversible ones. Another phenomenon observed from the numerical results was the occurrence of binary azeotropes isopropanol–water in the non-ideal mixture analyzed.

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### 1. Introduction

Distillation is one of the most important separation processes, mainly because it allows separating mixtures in large scale units. The separation of homogeneous and heterogeneous azeotropic mixtures is of great interest to industry, and a large number of such distillation columns are in operation. Furthermore, the need for developing new feasible sequences of distillation columns has increased to meet the demand for clean and economical processes.

The knowledge of the mixture behavior, in terms of its simple distillation path, is one of the most important tasks of the detailed separation process design [1,2]. For ternary and quaternary mixtures, this behavior can be represented in residue curve maps. Fien and Liu [3], Widagdo and Seider [4], and Kiva et al. [5] have presented reviews of the concepts and applications of residue curve maps. Kiva et al. [5] noted Russian publications on this subject as well as the history of residue curves. Manan and Alcántara-Bañares [6] published a catalog with some feasible separation sequences for homogeneous azeotropic distillation, based on residue curve map analysis.

In most works, residue curve maps have been calculated using the equilibrium stage model. There is some evidence, however, that the non-equilibrium model is able to make a better prediction of composition profiles in distillation columns than the equilibrium stage model [7]. The construction of residue curve

maps and dynamic simulations of distillation column using a non-equilibrium stage model has been intensively investigated [8–13]. It has also been accepted by [14,15] that the crossing of simple distillation boundaries is possible in some cases. It is important to analyze this conclusion more carefully, however, since the simple distillation boundaries are also composition trajectories and they may be affected by the model applied in their construction.

Silva et al. [9] developed another approach for the non-equilibrium model analysis, which took the dynamic behavior of simple batch distillation equipment into consideration. When it is performed under irreversible conditions, equilibrium becomes a local property, as stated by the microscopic reversibility principle [16] and the bulk properties of the phases are not related by thermodynamic equilibrium relationships. This approach is called “irreversible model”. In this model, only one factor, namely  $\alpha_i$ , is defined for correcting the non-equilibrium effects so that a compact expression for the vector composition of the vapor phase can be obtained, which takes into consideration vapor mass transfer coefficients for each component. Moreover, this model takes into account the existence of azeotropes as singular points. Schluender [17] gave the name of azeotropes to nodes different from those of pure components.

The objective of the present work is to calculate residue curve maps using the irreversible model developed by Silva et al. [9], which takes into consideration the dynamic behavior of a non-equilibrium simple batch distillation. A computational program, in Matlab language, was developed in order to calculate the composition trajectories. The methanol/isopropanol/water mixture was chosen as the case study.

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**Table 1**Influence of the parameters ( $A$ ,  $q$ ) in the irreversible factor average, with isopropanol in the steady state.

Irreversibility factor average	$A = 300 \text{ m}^2 q = 0.05 \text{ mol/s}$	$A = 15 \text{ m}^2 q = 0.05 \text{ mol/s}$	$A = 30 \text{ m}^2 q = 0.05 \text{ mol/s}$	$A = 30 \text{ m}^2 q = 0.005 \text{ mol/s}$	$A = 30 \text{ m}^2 q = 0.25 \text{ mol/s}$
$\alpha_1^a$	1.001670	1.034772	1.017071	1.001667	1.088983
$\alpha_2^a$	0.9997542	0.995329	0.997597	0.999754	0.989523
$\alpha_3^a$	1.0018976	1.039929	1.019485	1.001895	1.104502

<sup>a</sup> System methanol(1)–isopropanol(2)–water(3). These values of irreversible factor are average values of the  $\alpha_i$  taken along the residual curve.

## 2. Mathematical model

Thermodynamic topological analysis of distillation or residue curve map analysis was first developed by Gurikov [18]. Zharov [19] gave a more rigorous mathematical foundation to curve map analysis and expanded it to include multicomponent mixtures. Serafimov [20] proposed the use of structural information of vapor–liquid equilibrium (VLE) diagrams to predict feasible separations in continuous distillation. Following the Russian work, Doherty and Perkins [21] developed a set of nonlinear ordinary differential equations (Eq. (1)) to construct a residue curves map analysis:

$$\frac{dx_i}{d\xi} = x_i - y_i \quad i = 1, 2, \dots, c - 1 \quad (1)$$

where  $x_i$  and  $y_i$  are the liquid and the vapor mole fractions of component  $i$  in the bulk phase, respectively,  $c$  is the number of components, and  $\xi$  is a dimensionless time. Zharov [19] and Serafimov [20] used the opposite sign for the dimensionless time.

In order to integrate Eq. (1), it is necessary to find a relationship connecting the vapor and the liquid phase compositions. The two-film theory is used to correlate the bulk concentrations in both phases. Liquid and vapor compositions at interface are denoted by  $x_i^*$  and  $y_i^*$  and the compositions of the liquid and of the vapor in the bulk of the phases are denoted by  $x_i$  and  $y_i$ , respectively. The theory assumes, also, that all the resistance to the mass transfer is concentrated in the film region. The compositions in the liquid and vapor sides of the interface are assumed to be in equilibrium. This is required by the thermodynamic of irreversible processes, imposing a stricter requirement than the reversible theory does, that is, the infinitesimal subsystems are required to be in equilibrium at every instant [15].

Following this approach, Silva et al. [9] presented a set of differential equations given by

$$\frac{dx_i}{d\xi} = x_i - \alpha_i y_i^* \quad i = 1, 2, \dots, c - 1 \quad (2)$$

which is similar to the one developed by Doherty and Perkins [21], but allows for the mass transfer phenomena to be included in the parameter  $\alpha_i$ , because an essential phenomenon in simple batch distillation device is the net mass transfer of the component across the interface. It is impossible for such device to work without net mass transfer from liquid to vapor allowing the liquid vaporise. The development of this model is shown and detailed explanations are found in Silva et al. [9].

The parameter  $\alpha_i$  can be calculated by

$$\alpha_i = \frac{Ak_{i,\text{eff}}^V P^*}{RTq + Ak_{i,\text{eff}}^V P} \quad (3)$$

where  $q$  is the molar flow rate at which the vapor is withdrawn from the equipment,  $P^*$  is the total pressure at interface,  $P$  is the total pressure in the bulk of the vapor phase,  $A$  is the interfacial surface area of the mass transfer equipment,  $k_{i,\text{eff}}^V$  is the effective mass transfer coefficient of component  $i$  in the vapor film,  $R$  is the gas constant, and  $T$  is the absolute temperature of the system. In simple batch distillation there is bulk fluid motion across the film. The batch distillation process is a differential distillation,

where back-diffusion is not allowed to occur. Vapor is formed at the liquid–vapor interface across the film towards the bulk vapor driven by the pressure difference across the film. This difference may be generated by a vacuum system, by a heat exchanger, or by both. The existence of a pressure difference across the film is necessary for vapor outflow from the equipment. Doherty and Perkins [21] stated that the vapor stream is instantaneously removed from contact with the liquid, that is, at infinite velocity, which requires a very high pressure difference across the film.

As observed in Table 1, the irreversible factor is more sensitive the variation of the area interfacial than flow molar rate. As shown in Table 1, the irreversible factor tends to 1 (i.e. equilibrium) as larger the area interfacial or as smaller the molar flow rate. The parameter  $\alpha_i$  is unity using the assumptions of the Doherty and Perkins model [21], when  $q=0$ , i.e.  $P=P^*$ , since the reversibility of the process implies absence of net mass transfer. The parameter  $\alpha_i$  also becomes unity when  $k_{i,\text{eff}}^V$  has the same value for each component  $i$ , i.e.,  $k_{1,\text{eff}}^V = k_{2,\text{eff}}^V = \dots = k_{c,\text{eff}}^V$ . In these cases, an irreversible system is similar to a reversible one.

In order to calculate the parameter  $\alpha_i$ , it is necessary to estimate the effective mass transfer coefficients in the vapor phase for each component present in the mixture. For this purpose, Eq. (4) is applied, assuming a film thickness equal to 1 mm. Taylor and Krishna [22] proposed this value for the film thickness in a distillation example. Based on Doniec's studies [23], Nicolaiewsky et al. [24] developed an equation to estimate liquid film thickness for packed columns. Further work has investigated this and other correlations have been proposed [25] in order to predict film thickness values with less uncertainty,

$$k_{i,\text{eff}}^V = \frac{D_{i,\text{eff}}^V}{L} \quad (4)$$

where  $D_{i,\text{eff}}^V$  is the effective diffusion coefficient, and  $L$  is the film thickness.

Effective diffusion coefficients were calculated by Wilke's formula [26], according to

$$D_{i,\text{eff}}^V = \frac{1 - y_i}{\sum_{\substack{k=1 \\ k \neq i}}^c (y_k / D_{ik}^V)} \quad (5)$$

where  $D_{ij}^V$  is the binary mass transfer coefficient for components  $i$  and  $j$  in the vapor phase. Eq. (5) must be used when species  $i$  diffuse through a  $c - 1$  stagnant mixture of gases. In a simple distillation process, both gas and liquid are moving, and it is not strictly correct to take into consideration a stagnant gas phase. Despite this, Eq. (5) is the one most employed in the literature and it was the one used in the present work.

It was still necessary to estimate the binary diffusion coefficients. The correlation of Fuller et al. [27] was recommended by Taylor and Krishna [22],

$$D_{ij}^V = 0.01013T^{1.75} \frac{\sqrt{(M_i + M_j)/M_i M_j}}{P(v_i^{1/3} + v_j^{1/3})^2} \quad (6)$$

with  $T$  in K,  $P$  in Pa, and  $D_{ij}^V$  in  $\text{m}^2/\text{s}$ . In Eq. (6),  $v_i$  is the molecular diffusion volume of component  $i$  and it is calculated by summing

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