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Design of non-equilibrium stage separation systems by a stochastic optimization approach for a class of mixtures

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ABSTRACT

Design and analysis of distillation columns usually takes place by using rigorous equilibrium models, where efficiencies are utilized to enhance the designs obtained and have a better approach to the real performance of the column. A second alternative, based on the mass and heat transfer rates, has been proposed and it is known as the non-equilibrium (or rate-based) model. By employing this approach, the use of supposed values for efficiencies is not necessary. Nevertheless, to the authors' knowledge, there is not a short-cut design model for analysis of distillation columns with the non-equilibrium model. In this work, the design and optimization of conventional and intensified distillation sequences, with equilibrium and non-equilibrium models for the separation of ternary mixtures, is presented. The multiobjective optimization is performed by a stochastic technique with handling constraints, which is also coupled to a process simulator. This strategy allows analyzing the distillation systems with the complete rigorous models (MESH and MERSHQ equations, respectively). Optimal designs are then compared to determinate relationships between the design parameters of the optimal equilibrium sequences and the optimal non-equilibrium sequences. It has been found that the optimal on heat duty for each analyzed systems is almost the same for both, equilibrium and non-equilibrium models, but with different number of stages. Nevertheless, other design variables have only slight differences between models for an optimal structure.

1. Introduction

Distillation is one of the most used separation processes on chemical and petrochemical industries. It is a well-known process and its design and control has been studied since many years ago. Nevertheless, its main drawback is its inherent low second-law efficiency, which results into high external energy requirements. To enhance the energetic performance of distillation for ternary mixtures, the use of thermally coupled distillation systems has been proposed and analyzed; it has been showed that those schemes may be helpful to obtain energy savings of about 30% when compared to the conventional distillation sequences [1–7]. For difficult separations, the use of hybrid processes as extractive distillation has been proved as a good alternative for achieving high purities of the products. Such systems may have lower energy requirements and lower total annual costs than the conventional trains [8–10]. Design and analysis of distillation systems is usually performed by using the so-called equilibrium model, which considers that phase equilibrium is reached on each stage of the column. Nevertheless, equilibrium is rarely achieved on a real tray, thus, efficiencies are used to take into account deviations from the ideal performance of the tray. Since efficiencies are not known a priori, their values are supposed when designing a distillation column, and usually a single, constant value for efficiency is considered for all the trays in the column. This assumption may lead to under or over-designing the column. Thus, an alternative model was proposed by Taylor and Krishna, which considers the mass and heat transfer rates on each tray and assumes equilibrium

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Nomenclature

Q_i (kJ/h)	heat duty of the column i
Q_T (kJ/h)	total heat duty
N_i	number of stages of the column i
N_T	total number of stages
N_{EQ}	number of stages for the equilibrium model
N_{NEQ}	number of stages for the non-equilibrium model
F_{solv} (kmol/h)	molar flow rate of solvent
$\mathbf{y}_m$	vector of obtained purities for the m components
$\mathbf{x}_m$	vector of required purities for the m components

only on the interface [11] this model is known as non-equilibrium (NEQ) model. The successful use of the non-equilibrium model for the analysis of intensified sequences has been reported previously [12–15].

Agreement of the results obtained by simulations with the non-equilibrium model and experimental data has also been reported [15,16]. Different design and optimization methodologies have been proposed, such as parametric analysis [12,13], orthogonal collocation [17], simulated annealing [18,19] and differential evolution [20]. The aforementioned non-equilibrium optimization approaches consider just one objective, usually the total annual cost. In this work, a multiobjective genetic algorithm, with constraints handling, coupled to the process simulator Aspen Plus is used for the optimization of conventional and intensified distillation systems by using the equilibrium and the non-equilibrium model. The genetic algorithm is accelerated with artificial neural networks, as proposed by Gutiérrez-Antonio and Briones-Ramírez [21]. Furthermore, the genetic algorithm is linked to the process simulator Aspen Plus, thus the rigorous models of the systems are already available; and it can be used for the optimization. Optimal designs for both models are compared in terms of Pareto fronts, in order to obtain guidelines for the design of low-cost non-equilibrium distillation systems taking as a basis the equilibrium designs.

2. Case of study

In order to cover a representative range of analyzed mixtures, different components and compositions have been considered; with thermodynamic behavior ranging from ideal to non-ideal. Furthermore, ordinary and intensified distillation sequences have been studied. The distillation systems presented in this work can be grouped as follows:

- Ordinary distillation sequences (conventional and thermally coupled).
- Extractive distillation (conventional and thermally coupled).

The mixtures considered for separation in ordinary distillation sequences are shown in Table 1, together with the feed composition, recovery and desired purity. The first mixture consists of alcohols: methanol (MEOH), ethanol (ETOH) and butanol (BUOH); with two feed compositions: low and high composition of the middle-boiling component. This mixture will be separated on a conventional direct sequence (Fig. 1a) and a thermally coupled direct sequence (Fig. 1b). In Fig. 1, A, B and C represent the light, middle and heavy components, respectively. The second mixture consists of hydrocarbons with the presence of an isomer: isopentane (IC5), *n*-pentane (NC5) and *n*-hexane (NC6), with two different feed compositions. This mixture will be treated on a conventional indirect sequence (Fig. 1c) and a thermally coupled indirect sequence (Fig. 1d).

To consider mixtures far from ideality, systems with the presence of azeotropes have been studied. Those mixtures have been purified using extractive distillation to achieve high purities of the components. In Table 2, azeotropic systems analyzed in this work are presented. The first azeotropic mixture has acetone (ACET) and methanol (MEOH), for which a minimum boiling azeotrope has been reported at a composition of 77.6 mol% of acetone [22]. This mixture is separated in an extractive distillation direct sequence (both conventional and thermally coupled, Fig. 2a and b, respectively) using water as solvent to obtain purities higher than the azeotropic ones. The second azeotropic mixture consists on ethanol (ETOH) and water (H_2O), where a maximum boiling azeotrope exists between ethanol and water for purities higher than 90 mol% of ethanol (about 96 wt%) [23,24]. This mixture is also purified in an extractive direct sequence, using ethylene glycol as solvent. The trays for all the distillation systems (conventional, extractive and thermally coupled) are Sieve trays.

The stochastic optimization strategy used in this work is explained in Section 3.

3. Optimization tool

A multiobjective genetic algorithm with constraints handling [21] has been used for the optimization of the proposed distillation sequences. The genetic algorithm is coupled to the process simulator Aspen Plus, thus the whole equilibrium and

Table 1
Mixtures analyzed for ordinary distillation.

Mixture	Components	Feed composition (mol%)	Recovery (mol%)	Desired purity (mol%)
M1F1	Methanol	0.4	0.99	0.995
	Ethanol	0.2	0.98	0.961
	Butanol	0.4	0.99	0.995
M1F2	Methanol	0.15	0.99	0.955
	Ethanol	0.7	0.98	0.996
	Butanol	0.15	0.99	0.955
M2F1	Isopentane	0.4	0.99	0.995
	n-Pentane	0.2	0.98	0.961
	n-Hexane	0.4	0.99	0.995
M2F2	Isopentane	0.15	0.99	0.955
	n-Pentane	0.7	0.98	0.995
	n-Hexane	0.15	0.99	0.955