A Short Note on Steady State Behaviour of a Petlyuk Distillation Column by Using a Non-Equilibrium Stage Model

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A Petlyuk distillation column, considering equilibrium and non-equilibrium stage models, was studied. Rigorous simulations were conducted using Aspen Plus™ RATEFRAC Module for the separation of ternary mixtures. According to the equilibrium model, the energy-efficient design of the Petlyuk column requires that the intermediate component be extracted from the maximum point in the composition profile in the main column. It was found that, for the intermediate component, mass transfer occurs from the vapour to the liquid phase from the top of the column to the stage where the side stream is extracted, from this point mass transfer occurs in the opposite direction. This point, considering the non-equilibrium model, corresponds to the stage in which the net mass transfer rate is zero. For the case of two segments per stage, it was found that the heat duties predicted by the equilibrium model are significantly lower than those obtained by using the non-equilibrium model, which is consistent with previous reported results. However, it is important to say that despite the higher energy duty predicted by the non-equilibrium model; both models predict significant energy savings.

On a étudié une colonne de distillation de Petlyuk en considérant des modèles d'étage en équilibre et hors équilibre. Des simulations rigoureuses ont été menées au moyen du module RATEFRAC d'Aspen Plus™ pour la séparation de mélanges ternaires. Selon le modèle en équilibre, une conception énergétiquement efficace de la colonne Petlyuk nécessite que le composant intermédiaire soit extrait du point maximum du profil de composition dans la colonne principale. On a trouvé que, pour le composant intermédiaire, le transfert de masse se produisait de la vapeur vers le liquide de la tête de la colonne jusqu'à l'étage où le courant secondaire est extrait; à partir de ce point le transfert de masse se produit dans la direction opposée. Ce point, en considérant le modèle hors équilibre, correspond à l'étage où le taux de transfert de masse net est nul. Dans le cas où il y a deux segments par étage, on a trouvé que les rendements thermiques prédits par le modèle en équilibre étaient significativement plus faibles que ceux obtenus à l'aide du modèle hors équilibre, ce qui est cohérent avec les résultats existants. Cependant, il est important de préciser que malgré le rendement énergétique plus élevé prédit par le modèle hors équilibre, les deux modèles fournissent des économies d'énergie significatives.

Keywords: non-equilibrium distillation model, energy savings, Petlyuk column

INTRODUCTION

Distillation is the most widely used separation operation for most of the fluid mixtures. Unfortunately, not only do distillation columns require a large amount of energy to achieve the separation task (Tedder and Rudd, 1978), but also this separation technique is highly inefficient in its use because of its low thermodynamic efficiency (Flores et al., 2003). As a result, the search for energy-efficient distillation schemes is a current trend in process systems engineering. One way of reducing the energy demand in distillation is by using thermally coupled distillation sequences. An important effort has been focused on the development of new design and optimization methods for thermally coupled distillation columns, which can provide savings up to 30% of the total annual cost for the separation of some multicomponent mixtures, as compared to classical distillation sequences based on conventional columns (Triantafyllou and Smith, 1992; Hernández and Jiménez, 1999; Hernández et al., 2003; Rong et al., 2000; Blancarte-Palacios et al., 2003; Agrawal, 2000; Rong et al., 2003). Such coupled distillation sequences use thermal links that can be implemented by eliminating either a reboiler or a condenser and then introducing recycle streams in the vapour or the liquid phases, respectively. The most important thermally coupled distillation sequence is the Petlyuk column (fully thermally coupled), which uses a prefractionator linked by two recycle streams (Figure 1). The rationale behind this distillation sequence has been implemented in some chemical industries through the use of a thermodynamically

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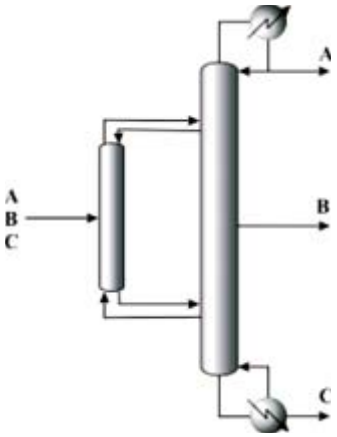

Figure 1. Petlyuk distillation column

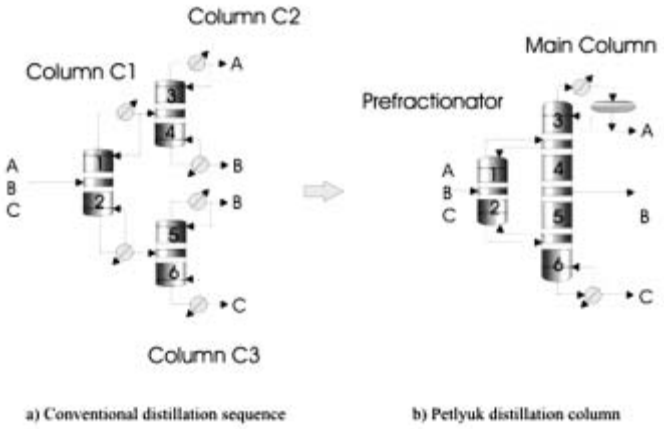

Figure 2. Design strategy of the Petlyuk column from a conventional distillation sequence

equivalent column consisting of a single shell and a dividing wall, and the reported savings in both energy and capital costs have been of around 30% (Kaibel and Schoenmarkers, 2002). Its thermodynamic efficiency has been attributed to the absence of remixing in the main column, i.e., the side stream is placed where the maximum concentration value of the composition profile of the intermediate component is located (Triantafyllou and Smith, 1992; Hernández et al., 2003). Design methods for the Petlyuk column must take this fact into account in order to guarantee the energy consumption reduction.

Most of the works related to the design, optimization and control of distillation columns use the equilibrium model approach, obtaining, for the case of the Petlyuk column, energy savings of up to 50%. However, no use of the non-equilibrium model approach has been made so far for the study of the Petlyuk column. As a result, the simulation of this column by using a rigorous non-equilibrium stage model is carried out in this work in order to understand its steady state behaviour.

The basic equations for the non-equilibrium model can be found elsewhere (e.g. Seader and Henley, 1998). These equations include phase mass balances, phase energy balances, equilibrium relations, summation equations, mass transfer rate in the vapour phase, mass transfer rate in the liquid phase, and energy transfer rate.

It is worth noting that some works regarding non-equilibrium stage model have been reported, but these works only deal with single columns. Important works were published by Krishnamurthy and Taylor (1985a, 1985b) in the 1980s. They used the non-equilibrium stage model in the simulation of distillation columns using some solution techniques based on Newton's method. They also compared their results with experimental data.

Taylor et al. (2003) extended the application of the non-equilibrium approach for the modelling of different distillation cases, and they found that this representation can convey more realistic results, even for complex distillation, e.g. reactive distillation, three-phase distillation, heterogeneous azeotropic distillation, etc.

Higler et al. (2004) applied the non-equilibrium model to the three-phase distillation case, including mass and energy balances for each of the three phases. They found that a non-equilibrium model is more suitable for this class of problems than the equilibrium model, even considering efficiency factors. A non-equilibrium model for three-phase distillation in packed distillation column was presented by Repke et al. (2004). Their model also took into account the mass transfer between all phases.

In this work, the application of the non-equilibrium stage model to the simulation of a Petlyuk distillation column is presented. The Aspen Plus™ RATEFRAC Module was used to obtain the composition profiles, mass transfer rates and optimum energy duty for this complex column. The Aspen Plus™ RATEFRAC Module uses the Chan and Fair, Scheffe and Weiland and Grester mass transfer correlations for sieve, valve and bubble cap trays, respectively. These mass transfer correlations are widely used in the non-equilibrium stage model (Taylor and Krishna, 1993).

DESIGN AND OPTIMIZATION METHODS

The energy-efficient design of the Petlyuk column was obtained using the equilibrium-based method described by Hernández and Jiménez (1999). The method is briefly depicted in Figure 2. The conventional distillation sequence shown in Figure 2a results from the use of the Fenske-Underwood-Gilliland shortcut distillation method, optimized by using the rigorous equilibrium stage model included in the Aspen Plus™ RADFRAC Module. The number of prefractionator stages shown in Figure 2b is equal to the number of stages in column C1 from Figure 2a (sections 1 and 2). The total number of stages in the main column of the Petlyuk sequence (Figure 2b) equals the summation of the stages in columns C2 (sections 3 and 4) and C3 (sections 5 and 6) shown in Figure 2a. Two recycle interconnecting streams are introduced in the Petlyuk sequence. The mass flow rate of both recycle streams is varied until the minimum energy requirement in the reboiler is found. This optimization strategy is explained in detail in the work of Hernández and Jiménez (1999). It is important to note that the optimized design of the Petlyuk column can be obtained using MINLP techniques (Grossmann et al., 2005).

CASE STUDY

To assess the application of the non-equilibrium stage model, the separation of two ternary mixtures were considered: mixture M1 (n-butane, n-pentane and n-hexane) and mixture M2 (benzene, toluene and styrene) for two molar compositions F1 (0.4, 0.2 and 0.4) and F2 (0.15, 0.7 and 0.15). Recoveries of up to 98.7%, 98% and 94%, respectively, were obtained for each component of the ternary mixture. Three different types of distillation trays were tested: sieve, valve and bubble cap. Operational pressures were set in advanced in order to guarantee the use of cooling

Table 1. Trays in each section in the distillation sequences for mixture M1 and feed composition F1

Conventional distillation sequence	Petlyuk column
Column C-1	Prefractionator
section 1 = 10	section 1 = 10
section 2 = 10	section 2 = 10
feed stage = 11	feed stage = 11
top pressure [atm] = 3.87	
Column C-2	Main column
section 3 = 8	section 3 = 8
section 4 = 8	section 4 = 7
feed stage = 9	section 5 = 9
top pressure [atm] = 4.30	section 6 = 7
	top pressure [atm] = 4.30
Column C-3	
section 5 = 9	
section 4 = 7	
feed stage = 10	
top pressure [atm] = 1.37	

water in the condensers. The operation conditions are shown in Table 1 for the case of mixture M1 and feed composition F1. A pressure drop of 0.68 atm for each column was assumed.

RESULTS

The study was conducted in two stages: in the first part, the design and optimization of the Petlyuk column were obtained by using a rigorous equilibrium stage model, whereas in the second part, the optimized design was tested through the use of the non-equilibrium stage model. Typical results are presented for the case of mixture M1 and feed composition F1.

The tray sections reported in Table 1 were determined through the use of the design and optimization method reported by Hernández and Jiménez (1999) assuming equilibrium operation. When the non-equilibrium stage model was used for the simulation of the Petlyuk column, an important aspect as noted in Figure 3 is that the side stream is obtained from maximum point in the concentration profile of the intermediate component (stage 17). This guarantees a good design with respect to the energy consumption (although it may not be the global optimum value).

Figure 4 shows the minimization of the energy consumption for the two recycle streams by using the non-equilibrium model. It is important to note that the optimization surface is very similar to that obtained using the equilibrium model, as reported in the work of Jiménez et al. (2003). The optimization was carried out considering two segments per each stage; this is in agreement with the work of Peng et al. (2002). Figure 5 shows small differences between the composition profiles for the intermediate component predicted by using the two models, but the same trends are observed.

Some important aspects are observed when the Petlyuk column is studied with the non-equilibrium model. For instance, in Figure 6 it can be observed that mass transfer occurs from the vapour to the liquid phase as we move from the top to the side stream tray and in the opposite direction from this to the bottom tray. In stage 17, the net mass transfer rate is zero, which corresponds to the maximum point in the composition profile shown in Figure 3. The net mass transfer rate for the lightest component occurs from the liquid to the vapour phase in the

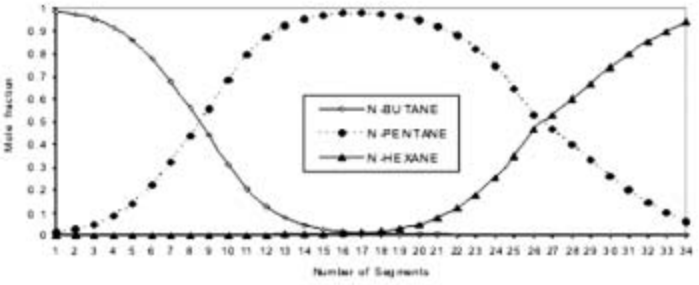

Figure 3. Concentration profiles in the Petlyuk column (non-equilibrium stage model) for mixture M1 and feed composition F1

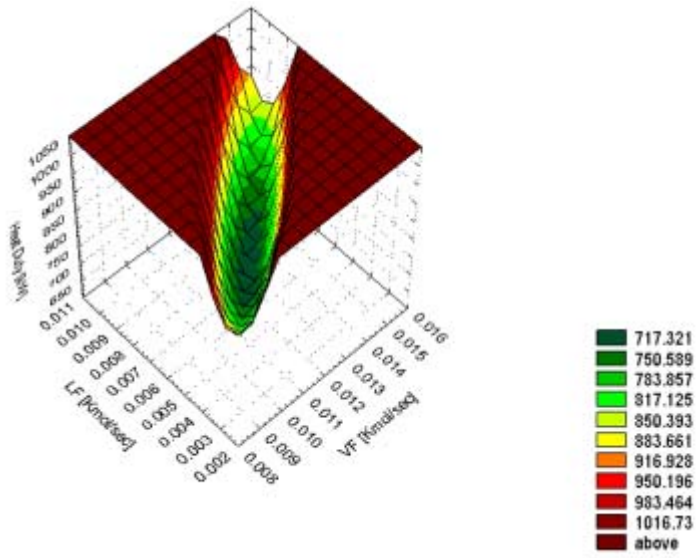

Figure 4. Optimization of the Petlyuk column (non-equilibrium) for mixture M1 and feed composition F1

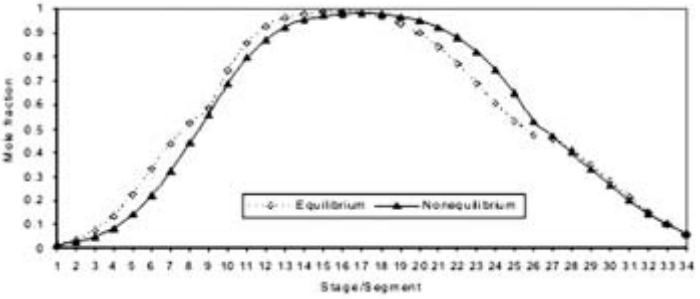

Figure 5. Composition profiles for the intermediate component considering equilibrium and non-equilibrium models for mixture M1 and feed composition F1

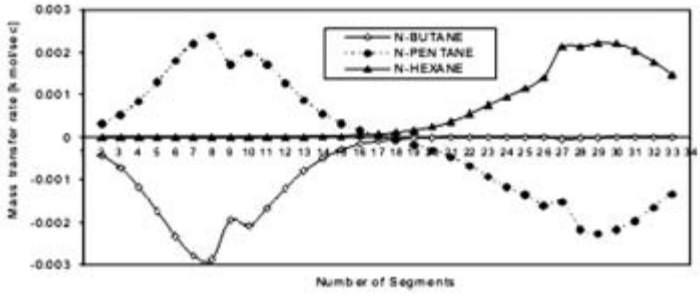

Figure 6. Mass transfer rates in the Petlyuk column (non-equilibrium) for mixture M1 and feed composition F1.

upper part of the column and it is zero in the lower part. For the case of the heaviest component, the net mass transfer is zero from the top to side stream stage, and it occurs from the vapour to the liquid phase in the rest of the column.

Since the effective mass transfer area is very important in the case of the non-equilibrium stage model, the influence of the column diameter on the energy consumption is shown in Figure 7. This behaviour is not predicted by the equilibrium stage model. In Figure 8, it can be observed that the energy consumption is a strong function of the type of plate, being the lowest for the valve plate.

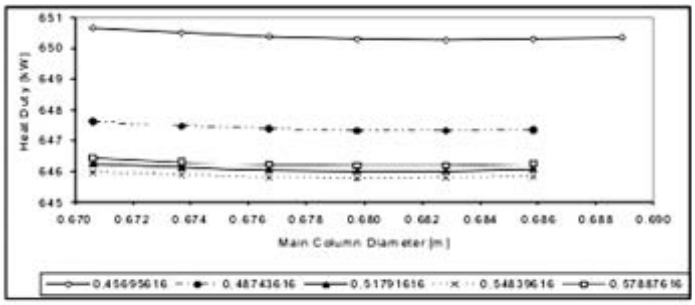

Figure 7. Influence of the column diameter in the energy consumption of the Petlyuk column for mixture M1 and feed composition F1 for five different diameters of the prefractionator column

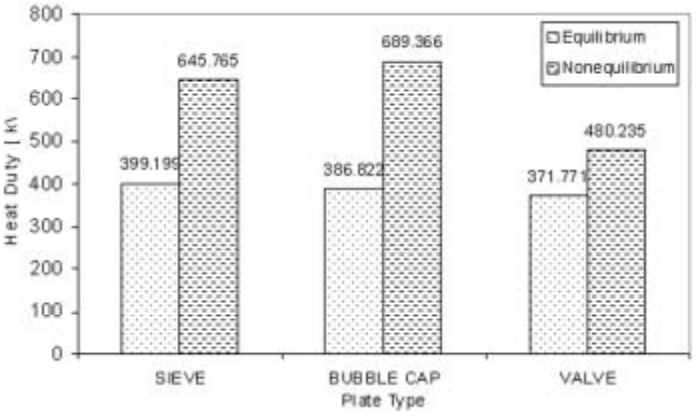

Figure 8. Effect of the type of plate in the energy consumption for mixture M1 and feed composition F1

Another important effect to be considered is the energy-performance of the Petlyuk distillation column and the conventional distillation sequence. In this sense, the equilibrium stage model predicts energy savings of up to 50% more for the Petlyuk distillation column than for the conventional sequence. The heat duties required for the separation indicated in the distillation sequences of Figures 2a and 2b using both, the equilibrium and the non-equilibrium models, are shown in Table 2. The results indicate that savings of around 50 and 30% for the Petlyuk column were predicted by using the equilibrium and non-equilibrium models, respectively. The heat duties are significantly lower when the distillation sequences are modelled by considering the equilibrium model; however, the values obtained by using the non-equilibrium model are more realistic. Finally, the results of the simulation of the Petlyuk column should be compared to those obtained in an experimental column.

CONCLUSIONS

In this work, a simulation of a Petlyuk distillation column and a conventional sequence for the separation of two ternary mixtures for two feed compositions are presented. The simulation was carried out using both the equilibrium and non-equilibrium stage models for sieve, valve and bubble cap trays. The results indicate that both stage models predict significant energy savings and that the energy consumption depends strongly on the interconnection recycle streams. However, the equilibrium model predicts heat consumptions significantly lower than those obtained by assuming non-equilibrium operation, the later being more realistic. The dependence of the energy consumption on the diameter of the distillation column can only be predicted by the non-equilibrium stage model. It is important to note that the side stream in the main column for the Petlyuk sequence should be placed where the maximum point in the composition profile for the intermediate component is located. In the case of the non-equilibrium stage model, this point corresponds to the zero net mass transfer rate.

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Table 2. Energy consumptions (kW) considering equilibrium and non-equilibrium models

Model	Conventional distillation sequence (Figure 2a)	Petlyuk column (Figure 2b)	Energy savings (%)
M1, F1			
Equilibrium	825.69	399.2	51.6
Non-equilibrium	1067.53	645.76	39.5
M1, F2			
Equilibrium	717.28	481.75	32.8
Non-equilibrium	1025.81	698.02	31.9
M2, F1			
Equilibrium	1531.97	670.20	56.2
Non-equilibrium	3322.28	1689.00	49.2
M2, F2			
Equilibrium	1162.13	721.64	37.9
Non-equilibrium	1833.87	1019.26	44.4

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