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Thermodynamic Analysis and Hydrodynamic Behavior of a Reactive Dividing Wall Distillation Column

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A complete thermodynamic analysis of a reactive dividing wall distillation column and an equilibrium reactor followed by a dividing wall distillation column was conducted for several equilibrium reactions using data of a real pilot plant for the distillation column. In addition, several aspects related to the hydrodynamic behavior of the implemented reactive dividing wall distillation column were analyzed in order to prevent operation problems with regard to hydraulics.

Results indicate that the reactive dividing wall column presented both higher thermodynamic efficiencies and lower exergy losses than those obtained in the classical configurations of a reactor plus a distillation column. The reactive dividing wall distillation column also required lower energy consumption compared to that required by classical processes. These facts confirm the higher energy efficiency of reactive dividing wall designs. Results also indicate that the reactive dividing wall column meets process intensification goals: i) it requires lower energy consumption, which can be translated into lower carbon dioxide emissions, and ii) the reduction in energy consumption can be associated with lower traffic of liquid in the column and reduction in column diameter (miniaturization). Finally, it was observed that proper collection of the liquid in a side tank and an adequate split to both sides of the dividing wall play an important role in hydraulics. The manipulation of this split enables minimum energy consumption and high thermodynamic efficiency.

1. Introduction

Current process design in chemical engineering must take into account aspects of process intensification such as miniaturized equipment, multipurpose equipment, minimum energy consumption, safe operation and environmental impact. A great deal of attention is currently being given to these important aspects in chemical engineering. For example, in a chemical plant, energy consumption in a separation process such as

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distillation can reach 40% of total consumption; hence, researchers in the field of distillation are developing new configurations that are capable of reducing both energy consumption and carbon dioxide emissions.

One alternative that has been explored is the use of thermally coupled distillation sequences, which can achieve energy savings of between 30 and 50% over conventional distillation sequences for the separation of some multicomponent mixtures (Tedder and Rudd, 1978; Hernández and Jiménez, 1999; Mascia et al. 2007; Rong and Turunen, 2006). These energy savings have been predicted using steady state simulation and mathematical programming, and their theoretical control properties and dynamic behavior have also been determined (Serra et al. 2003; Cárdenas et al. 2005). In this sense, dynamic responses under the action of feedback controllers obtained in thermally coupled distillation can be better than those of conventional distillation sequences. Based on these studies, practical implementation of thermally coupled distillation sequences has been conducted using dividing wall columns (Figure 1).

Along the same lines, reactive distillation is considered to be the most representative intensification operation because it combines reactions and separation in a single process unit. For the case of equilibrium reactions with products that can exhibit azetropic behavior, reactive distillation may be used for two reasons: i) conversion can be increased since the products are removed as they are formed, and ii) conditions are changed by the reaction and the azeotrope point does not appear.

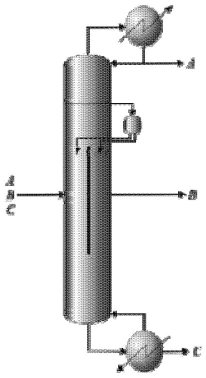
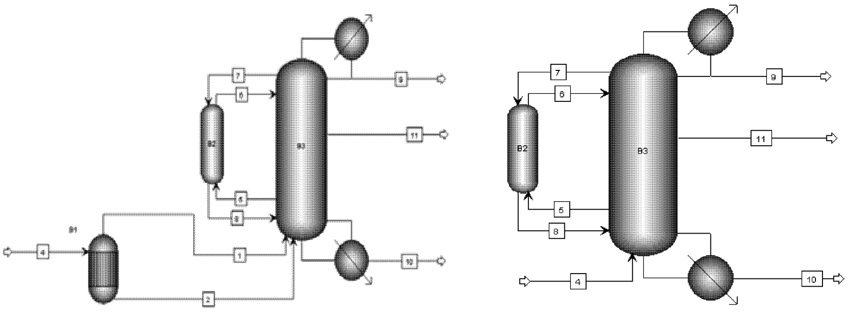


Figure 1 Dividing wall distillation column for ternary separations.

In this study, we present a thermodynamic comparison between reactive dividing wall distillation columns and classical processes involving a reactor followed by a distillation column. The comparison is made in terms of second law efficiencies and energy consumptions. Three equilibrium reactions were studied considering the two alternatives indicated in Figure 2, using Aspen Plus One^{TM}. The data for the reactive dividing wall distillation column under study correspond to a real pilot plant. Finally, several aspects related to the hydrodynamics of the reactive dividing wall distillation column are presented in order to demonstrate that the reactive distillation system does not present hydraulic problems.

2. Methodology

As indicated in the previous section, we studied equilibrium reactions considering two complex schemes. The first scheme involves the use of a reactor and a distillation column, and the second one uses a reactive fully thermally coupled distillation column that is thermodynamically equivalent to the dividing wall distillation column (Hernández et al. 2006). The schemes were optimized and simulated in Aspen Plus One^{TM} and are depicted in Figure 2. The design was obtained using the RADFRAC module of Aspen Plus. In the case of the reactive dividing wall distillation column, the design and optimization procedures are more complicated (Hernández and Jiménez, 1999) and require an initial tray structure based on a conventional distillation sequence and detection of the minimum energy consumption of the reactive dividing wall distillation column. As indicated in Figure 2, the two recycle streams are varied until minimum energy consumption in the reboiler is obtained.



(a) Reactor plus column (b) Reactive dividing wall distillation column

Figure 2 Schemes used to carry out the three equilibrium reactions.

With the optimized designs of the two schemes, the thermodynamic efficiencies can be obtained using the laws of thermodynamics. The following equations were taken from the textbook of Seader and Henley (2006).

First law of thermodynamics:

$$\sum_{\text{out of system}} \left(nh + Q + W_S\right) - \sum_{\text{in to system}} \left(nh + Q + W_S\right) = 0 \tag{1}$$

Second law of thermodynamics:

$$\sum_{\text{out of system}} (ns + Q/T_S) - \sum_{\text{in to system}} (ns + Q/T_S) = \Delta S_{irr} \tag{2}$$

Exergy balance:

$$\sum_{\text{in to system}} \left[nb + Q\left(1 - \frac{T_0}{T_S}\right) + W_S\right] - \sum_{\text{out of system}} \left[nb + Q\left(1 - \frac{T_0}{T_S}\right) + W_S\right] = LW \tag{3}$$

Minimum work of separation:

$$W_{min} = \sum_{\text{out of system}} nb - \sum_{\text{in to system}} nb \tag{4}$$

Second law efficiency:

$$\eta = \frac{W_{min}}{LW + W_{min}} \tag{5}$$

where $b = h - T_0 s$ is the exergy function, $LW = T_0 \Delta S_{irr}$ is the lost work in the system and η is the thermodynamic efficiency. The thermodynamic properties required in equations 1-5 were evaluated using the Aspen Plus One^{TM} process simulator. The analyzed reactive systems are indicated in equations 6-8, for the two schemes shown in Figure 2.

Ethanol + Acetic Acid ↔Ethyl Acetate + Water (6)

Methanol + Isobutylene ↔ Methyl tert-Butyl-Ether (7)

Ethanol + Ethylene Oxide ↔ Ethoxyethanol (8)

3. Results

Figure 3 shows a representative search of minimum energy consumption for the reactive dividing wall distillation column of Figure 2b, for Reaction 6. According to Figure 3, the energy consumption (QR) depends on a proper selection of the values of the two interconnecting liquid and vapor flows (FL and FV). Table 1 presents the optimum energy consumptions and second law efficiencies for the two schemes shown in Figure 2, for the three equilibrium reactions. The optimal energy consumptions and thermodynamic properties such as enthalpies and entropies are obtained using the process simulator Aspen Plus One^{TM}, and second law efficiencies are calculated using equations 1-5.

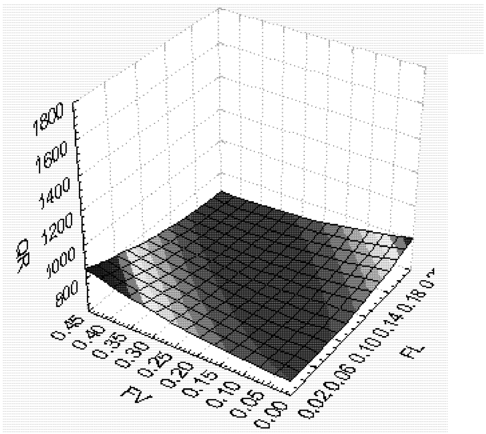


Figure 3 Search for optimal heat duty supplied to reboiler.

Table 1 Optimum energy consumptions and second low efficiencies.

Reaction	Scheme 2a	Scheme 2b	Scheme 2a	Scheme 2b
	Energy consumption (kW)		Second law efficiencies (%)	
1	4.51	2.85	11.56	15.30
2	3.50	1.37	24.76	39.66
3	9.41	7.77	25.79	28.17

According to Table 1, energy consumptions of the reactive dividing wall column are significantly lower than those of the classical process of an equilibrium reactor plus a separation on a dividing wall distillation column. This fact can be associated to internal heat integration in the reactive dividing wall distillation column leading to a reduction in total energy consumption of the reactive distillation scheme. When second law efficiencies are compared, it can again be noted that internal heat integration leads to higher thermodynamic efficiencies because of a reduction in energy demand in the reboiler. After thermodynamic analysis is conducted, an important aspect to be taken into account in the operation of the reactive dividing wall distillation column is a proper distribution of liquid and vapor in the section of the dividing wall, since it has been proven that this split plays an important role in energy consumption (Figure 3). In practice, it is difficult to manipulate both interconnecting flows; for that reason, the interconnecting vapor flow is fixed with the position of the wall, while the interconnecting liquid flow can be manipulated using a side tank (Figure 4). The manipulation and redistribution of the liquid prevent operational hydraulic problems such as poor distribution of liquid, and energy efficiency in the reactive distillation can be achieved.

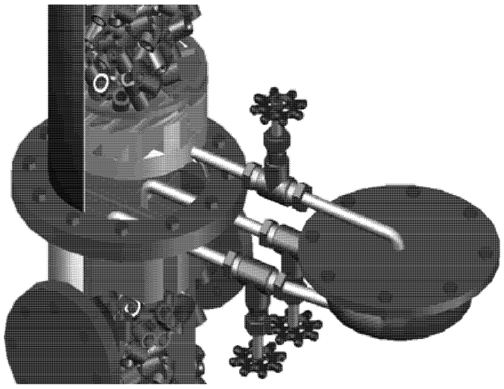


Figure 4 Side tank used in the reactive dividing wall distillation for proper operation.

4. Conclusions

A second law analysis and an operational study were conducted for a reactive dividing wall distillation column and a classical process of reactor plus a distillation column for several equilibrium reactions. Results indicate that the reactive dividing wall columns presented both higher thermodynamic efficiencies and lower energy consumptions than those obtained by the classical configurations of a reactor plus a distillation column. These facts confirm the higher energy efficiency of reactive dividing wall designs. Results also indicate that the reactive dividing wall column meets process intensification goals, i.e., energy consumption savings, reductions in carbon dioxide emissions, and miniaturization through reduction in liquid traffic. In addition, in order to achieve these benefits associated with internal heat integration, proper traffic of liquid and vapor in the section of the dividing wall is required.

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