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Heat Integrated Reactive Distillation Column (r-HIDiC): Implementing a New Technology Distillation

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Currently, several heat integration techniques have been studied, e.g. HIDiC column, showing a diminution in energy consumption in relation to conventional distillation column. In this work, an approach for process intensification in distillation columns is studied by merging both reactive distillation and heat integrated distillation column principles, resulting in the heat integrated reactive distillation column (r-HIDiC). A simulation study has been performed in order to compare the performance of reactive distillation column and r-HIDiC column in the synthesis of tert-amyl methyl ether (TAME). It was found that due to internal energy integration, the r-HIDiC column achieves a better performance with energy saving around 8%. In addition, it can be seen that the possibility of r-HIDiC column to operate at different pressures between the rectifying and stripping sections permits to overcome separation limitations resulting from presence of azeotropes.

1. Introduction

In chemical and petrochemical industry, separation operation is widely used to obtain products with high purity and aiming waste reduction. To improve the efficiency of the distillation column, several techniques for process intensification have been proposed. By combining two operations (reaction and separation) into a single vessel, reactive distillation has demonstrated its potential for capital productivity improvements, selectivity improvements, reduced energy use, and the reduction or elimination of solvents in the process (Hao-Yeh et al., 2010). On the other hand, to improve the energy efficiency by reducing the reboiler and condenser duties, various heat integration schemes have been proposed (Nakaiwa et al., 2003). Currently, a novel idea for process intensification by merging reactive distillation and heat integration principles, resulting in the heat integrated reactive distillation column (r-HIDiC), is increasing (Hao-Yeh et al., 2010; Santosh and Amiya, 2009). In this work, the concept of column r-HIDiC and its performance is studied in the synthesis of tert-amyl methyl ether (TAME). A comparison with the conventional reactive distillation column is made. The simulation study is performed using commercial software Aspen Plus 7.1, allowing understanding the operation of the column and presenting the potential of r-HIDiC in decreasing energy consumption.

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2. Concept of Heat Integrated Reactive Distillation Column

The basic concept of heat integration consists on the utilization of hot process streams to exchange heat with cold process streams. Although several heat integration techniques have been proposed, in this work, it is studied the internally heat-integrated distillation column (HIDiC). In this configuration, the heat transfer from de rectifying section to the stripping section leads the rectifying section to operate at higher pressure and temperature. The heat required to evaporate the liquid in the stripping section is obtained from the rectifying section, which decrease the energy charge on the reboiler. Recently, different works has been developed through computational tools (Jeffrey et al., 2010a-b) in order to understanding of fluid dynamics within of the HIDiC column. A schematic diagram of the concentric stage concept is shown in Figure 1(a).
Despite an increasing interest in the heat integration techniques and in the column control, the novel idea of locate a reactive zone placed in the HIDiC column in the specified stage range leads to a significant reduction of the capital and operating costs by combining both reaction and distillation processes in a single vessel, eliminating one process unit (Jie et al., 2009). In addition, applicability for mixtures with minimum and maximum boiling azeotropes can be processed in this configuration while reducing energy consumption. The configuration of r-HIDiC column is shown in Fig 1(b).

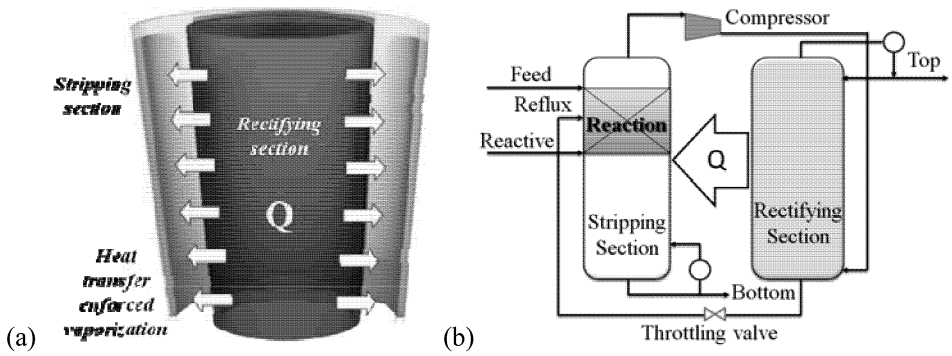

Figure 1: (a) Concept of concentric HIDiC, (b) Configuration of r-HIDiC.

3. Case Study: TAME Process and Chemical Kinetics

In this study, a quantitative comparison of the performance of conventional reactive distillation column and r-HIDiC column for the production of tert-amyl methyl ether (TAME) was carried out. TAME is an oxygenate that is used in gasoline blending as replacement for lead. The interest in TAME increased after bans on the use of methyl tertiary butyl ether (MTBE) because of environmental concerns (Muhammad and William, 2004). TAME is produced by reacting isoamylenes [2-methyl-1-butene (2M1B) and 2-methyl-2-butene (2M2B)] with methanol. The three main reactions that take place according to Muhammad and William (2004) and considered in this study are presented below. The reaction rates for the forward and reverse kinetics are given by Muhammad and William (2004).

2M1B + Methanol ↔ TAME (etherification) (1)

2M2B + Methanol ↔ TAME (etherification) (2)

2M1B ↔ 2M2B (isomerization) (3)

In this study, the column configuration (reactive zone, holdup, number of stage, pressure, temperature, reboiler and condenser) for conventional reactive distillation column proposed by William (2005), was used. It is assumed that the kinetics reactions occur in the liquid phase for the equilibrium conversion.

3.1 Reactive distillation process

Simulation studies were developed using the commercial software Aspen Plus 7.1 for steady state. The same design parameters of conventional reactive column for TAME process were used for developing the r-HIDiC column simulation. The reactions were described in the format of power-law. The forward and backward kinetic parameters used for this simulation, such as preexponential factors and activation energies, were published by Muhammad and William (2004).

3.2 Reactive column (R-HIDiC)

This simulation process is developed for an approximate configuration of heat integrated distillation column using Aspen Plus 7.1. Because it is a new configuration, the conventional software has not it in the model library, so strategies of simulation and short cut methods were developed for implementing the new technology. The concept of Heat Integrated Reactive Distillation Column is then established in the commercial simulator and results are presented in this study. In the new intensification system, reaction occurs in the specific area of the stripping section. The difference of pressure in this configuration presents possibilities for analyzing azeotropic mixtures. At the top of the rectification section, IC5 is obtained along with a significant amount of methanol due to the presence of azeotrope. In the simulation, internal heat integration takes place by a thermally inter-coupled arrangement established in the column.

4. Simulation Study

The TAME process was performed in two simulations. The first one related to the conventional reactive distillation (RC) and the second implements the technology of Heat Integration for r-HIDiC. The feed parameters are specified in Table 1.

Table 1: Design parameters of RC and r-HIDiC.

Item	RC	r-HIDiC	Item	RC & r-HIDiC
Stages	36	18/18	Composition	(mol fraction)
Rectifying (MPa)	4	10	MeOH	0.153
Stripping (MPa)	4	4	2M2B	0.011
Reacting Stages	7-13	8-16	TAME	0.102
Feed flow (kmol/h)	1230	1230	IC5	0.408
Reactant	Methanol	Methanol	Inert	0.326

The simulation was developed for steady state, using equilibrium stage model, heat is totally transferred, and it was not considered pressure drop in the column. The heat is transferred through the stream stages, so that a heat transfer is constant along the r-HIDiC column. In addition, the compressor was isentropic and the throttle valve is adiabatic in order to maintain the pressure in the system. The UNIFAC method was used for property calculations in both systems. The process was modeled assuming perfect mixing and azeotropic convergence.

5. Results and Analyses

In this work, the mixed IC5 fed to the column consists of 2M1B, 2M2B, n-pentane, i-pentane, 1-pentene, and 2-pentene (cis). The bottom product from both conventional reactive column and r-HIDiC column is high-purity TAME. Because the existence of azeotropes between methanol and all IC5 components, the distillate product is about 30 mol % methanol and 70 mol % inert IC5 in the conventional reactive distillation. Based on Figure 2(a), the pressure difference between the rectifying and striping sections in the r-HIDiC column improves the component concentration in the product streams of the separation process, because the r-HIDiC column proceed as a type of pressure-swing process. Figure 2(a) shows the T-x-y diagram for i-pentane/methanol at the pressure operation of r-HIDiC column: 4 bar for the stripping section and 10 bar for the rectifying section. It can be seen that the methanol composition of the azeotrope increases as the pressure increase.

The r-HIDiC column composition profiles are shown in Figure 2(b). The compression ratio between stripping and rectifying section is 4:10, respectively. This configuration permits to obtain a bottom purity of 91 mol % TAME in the stripping section. In the distillate, IC5 was obtained at 86 mol % at the top of rectifying column. Reboiler duty and condenser heat removal are 39.77 and 40.53 MW, respectively. As can be seen in Table 2, the r-HIDiC presents a decreasing in the energy consumption in comparison with a conventional reactive distillation column, which leads to a potential reduction of the operating cost.

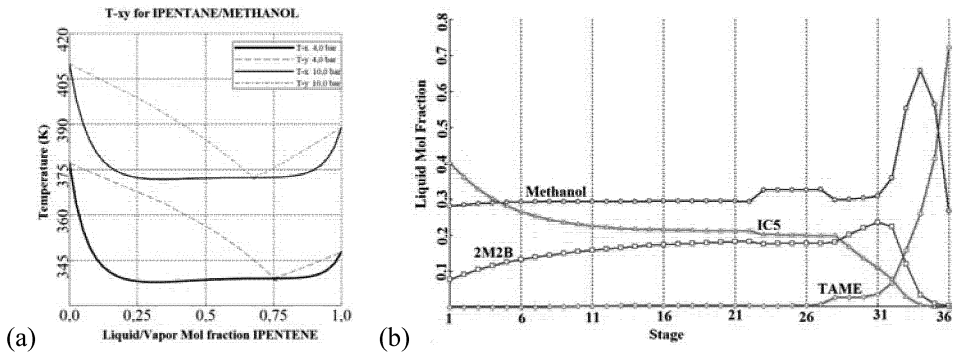

Figure 2: (a) T-xy diagram of TAME process, (b) Composition profiles in the r-HIDiC.

Figure 3 shows temperature profile for reactive distillation column and r-HIDiC column. The flat temperature and composition profiles in the reactive zone indicate the absence of significant vapour-liquid mass transfer as mentioned by Hoshang and James (1999). The parameters for set simulation of the reactive distillation and the r-HIDiC column were the same, in order to direct evaluation between these intensified processes. These results show that the implementation of intensified process for distillation, r-HIDiC column, is possible and requires experiences in both pilot and industrial scale.

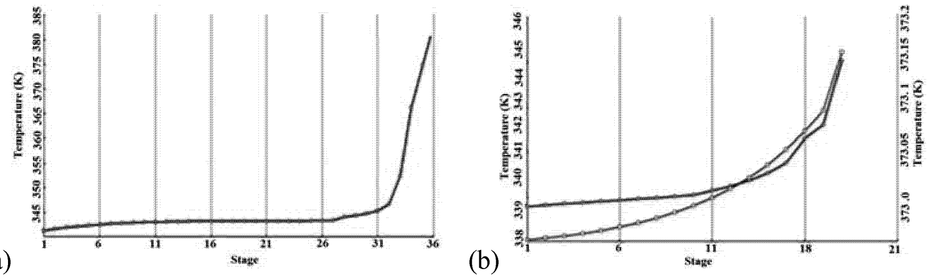

Figure 3: (a) Temperature profile RC, (b) Temperature Profile r-HIDiC.

Table 2: Results of conventional RC and r-HIDiC column.

Item	RC	r-HIDiC
Reboiler (MW)	43.15	39.77
Condenser (MW)	-43.64	-40.53
Boilup Rate (kmol/h)	4977	5613
Boilup Ratio	25.18	3.85
Reflux Ratio	4	4

6. Conclusions

In this work, simulation studies were developed in order to specify the feasibility of implementation of the new technology, reactive distillation with internal heat-integration, r-HIDiC column. Very few studies about this technology are available in the open literature. This intensified process merges the reactive distillation principles with heat integration techniques in distillation process for TAME synthesis. The simulations were performed using the commercial simulator Aspen Plus 7.1. The r-HIDiC column shows a diminution in the energy consumption of the order of approximately 8.0 % in relation to the conventional reactive column. The application of r-HIDiC column in the TAME process presents great advantage for azeotropic separation, owing at the difference of operation pressure in the two section of the r-HIDiC column, increasing the possibility to obtain purer components. The reaction takes place in the stripping section, which allows to the take advantage of heat present in the rectifying section, reducing the power consumption required by the reboiler. It was demonstrated that internal arrangements in distillation process is really effective for process intensification. Not only can product concentration be improved substantially, but also the capital investment in complexities process can be further reduced.

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