19th European Symposium on Computer Aided Process Engineering – ESCAPE19
J. Jeżowski and J. Thullie (Editors)

Design of Reactive Distillation with Thermal Coupling for the Synthesis of Biodiesel using Genetic Algorithms

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Abstract

The esterification of lauric acid and methanol is explored using a thermally coupled distillation sequence with a side rectifier and the Petlyuk distillation column. The study was conducted using as a design tool a multi objective genetic algorithm with restrictions.The product of the esterification can be used as biodiesel. It was found that the thermally coupled distillation sequence involving a side rectifier can produce biodiesel with a high purity (around 0.999) and also pure water, and the excess of methanol is recovered in a side rectifier. The results indicate that the energy consumption of the complex distillation sequence with a side rectifier can be reduced significantly by varying operational conditions. These reductions in energy consumption can be interpreted as reductions in carbon dioxide emissions.

Keywords: reactive distillation, biodiesel, genetic algorithm, energy consumption

1. Introduction

Due to increased energy demand and environmental concerns worldwide, important research is currently underway on biofuels and alternative energies, e.g., biodiesel, biomass, bioethanol. In the case of biodiesel, it has been reported that its production can be competitive with fossil diesel when the price of crude oil reaches USD 100 per barrel [1]. As a result, important process intensification polices have been taken into account in the design of new processes, due to reduction in oil reserves, and for minimization of carbon dioxide emissions and use of alternative energies. Attention has been paid to these important aspects in the process systems engineering area of chemical engineering. For example, in a chemical plant, energy consumption in a separation process such as distillation can be up to 40% of total consumption. As a result, researchers in the field of distillation are developing new configurations that can be capable of reducing both energy consumption and carbon dioxide emissions [2]. One alternative that has been explored in detail is the use of thermally coupled distillation sequences (TCDS) that can achieve energy savings between 30 and 50 percent over conventional distillation sequences for the separation of some multicomponent mixtures. These energy savings have been predicted using steady state simulation and mathematical programming; also, their theoretical control properties and dynamic behavior have also been determined [3]. Based on these studies, practical implementation of thermally coupled distillation sequences has been conducted using dividing wall columns.

Reactive distillation is considered to be the most representative intensification operation because it combines reactions and separation in a single process unit. As a result, TCDS options can be used to carry out reactions of esterification of fatty organic acids, and the produced esters can be used as biodiesel. This leads to important processes to produce biofuels using complex distillation systems that can reduce energy consumption, capital costs, and carbon dioxide emissions. Thus, in this paper, the production of biodiesel by esterification of methanol and lauric acid is studied using a thermally coupled distillation sequence with a side column and the fully thermally coupled distillation sequence. We have selected these distillation sequences because, for the separation of ternary mixtures, there are two types of thermally coupled distillation sequences: TCDS with side columns and the fully thermally coupled distillation sequence (Petlyuk distillation sequence). The schemes are depicted in Figure 1.

2. Strategy solution

In order to optimize the thermally coupled reactive sequences we used the multiobjective genetic algorithm with constraints coupled to Aspen Plus, developed by Gutiérrez-Antonio and Briones-Ramírez [4]. Their algorithm manages the constraints using a multiobjective technique based on the concept of non dominance proposed by Coello-Coello [5].

For the reactive thermally coupled systems the optimization problem includes as objectives the minimization of the total number of stages, the size of the reactive section and the heat duty of the sequence, but it also considers the interconnection flows:

$$\begin{aligned}&\text{Min } (Q_i, N_i, N_R) = f(R_i, N_i, N_{F,i}, N_{r1}, N_{r2}, F_k, N_k)\\&\text{subject to}\\&\vec{y}_m \geq \vec{x}_m\end{aligned} \qquad (2)$$

Where R_i is the reflux ratio, $N_{F,i}$ is the number of the feed stage and N_i is the number of stages of the column i of the sequence, N_{r1} and N_{r2} are the initial and final stages of the reactive section N_R in the column j, $\vec{y}_m$ and $\vec{x}_m$ are vectors of obtained and required purities for the m components, respectively. F_k and N_k are the value and location of the interconnection flow k.

In the reactive thermally coupled distillation sequences, there are four objectives to minimize: the number of stages in each column, the size of the reactive section and the heat duty of the sequence. For the sequences the objectives are in competition, so they have to be optimized simultaneously. The manipulated variables include reflux ratio, total number of stages, value and location of the interconnection flows, and size of the reactive section.

For the thermally coupled reactive distillation sequences we used 2000 individuals and 40 generations as parameters of the algorithm. These parameters were obtained through a tuning process, where several runs of the algorithm were performed with different number of individuals and generations.

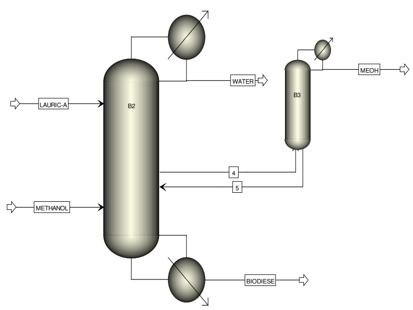
3. Case study

The esterification process can be represented conceptually by equation 3.

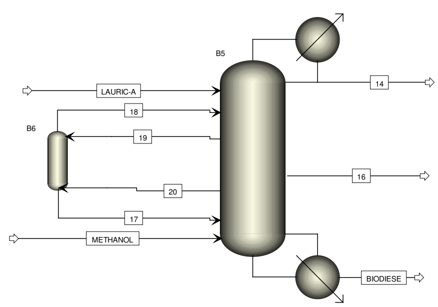
$$\text{Alcohol} \quad + \quad \text{Fatty Acid} \longleftrightarrow \text{Ester} \quad + \quad \text{Water} \tag{3}$$

This equilibrium reaction can be favored if the products are removed as the reaction proceeds. An additional problem may present itself, depending on the acid and the alcohol used, as binary or ternary homogeneous azeotropes can be formed in the reactive system. For highly nonideal systems, heterogeneous azeotropes can be formed. These key factors must be considered to select the appropriate thermodynamic model when the system is studied with process simulators. For this class of reactive systems, thermodynamic models such as NRTL, UNIFAC or UNIQUAC can be used to calculate vapor-liquid or vapor-liquid-liquid equilibriums.

The systems include two feed streams; the first is lauric acid with a flow of 100 lb-mol/h as saturated liquid at 1.5 bar, and the second is methanol with a flow of 120 lb-mol/h as saturated vapor at 1.5 bar. The reactive system is catalyzed using sulphuric acid. A mass fraction of 0.999 was assumed for the purity of the biodiesel stream.



(a) Reactive TCDS with a side rectifier.



(b) Reactive Petlyuk column.

Figure 1. Reactive TCDS for the production of biodiesel.

4. Results

The composition profiles of the optimized designs were analyzed in order to determine biodiesel composition. This is very important because the amount of acid is critical in motor vehicles. Figure 2 presents the composition profiles in the liquid phase for the reactive TCDS with side rectifier, as a representative profile of the analyzed reactive systems.

In the case of the reactive TCDS option with side rectifier, it is observed that it is possible to obtain almost pure biodiesel as the bottom product of the main column (mass fraction equals 0.999). In the distillate product of this column, the water produced in the reaction is removed, and the excess of methanol is recovered in the side rectifier column. This methanol, of course, could be returned to the reactive distillation column in order to obtain a more efficient reactive distillation process. When the composition profiles for the Petlyuk distillation column are analyzed, a similar result is obtained in terms of the purity of the biodiesel.

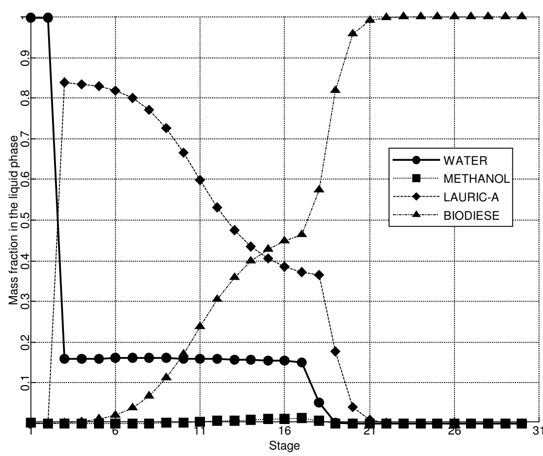


Figure 2. Composition profiles in the liquid phase of the main column of the reactive TCDS with a side rectifier.

For these complex reactive distillation sequences, Pareto front includes the complete set of optimal designs that satisfy the required purities: from minimum reflux ratio to minimum number of stages, and all designs between them. In this way, the engineer can establish the proper tradeoff between energy and equipment according to his particular needs, both actual and future. In this study, we choose the optimal values of 1059 and 4083 kW, for the reactive TCDS with side rectifier and the reactive Petlyuk column respectively, since, for us, they represent a good compromise between the objectives.

Regarding environmental aspects, Kencse and Mizsey [6] have reported that, in fact, gas emissions are directly linked to energy consumption since, in the chemical industry, the energy required in distillation is obtained from crude oil. As a result, reductions in energy consumption can be translated into reductions in carbon dioxide emissions. This important fact can be observed in Figure 3. According to Figure 3, the carbon dioxide emission can be incremented significantly when the operational conditions are different to those corresponding to the optimum. This point is important, because in terms of control and operational aspects, it has been reported [7] that the control properties of coupled schemes can be improved when the operational conditions fall outside the optimum. This is important because in the selection of the operational conditions, the engineer must take into account the fact that savings in carbon dioxide emissions can be achieved with more efforts in the control system.

Finally, regarding recent advances in the use of dividing wall distillation columns, it is possible to propose a single distillation column using a dividing wall and a side condenser. Additionally, this idea leads to reductions in capital costs. The proposed scheme is shown in Figure 4. This complex distillation scheme must be subjected to a control study in order to anticipate potential operational problems for set point tracking and load rejection. This topic is currently under study, but it is needed a kinetic model to obtain a dynamic model of the reactive system [8].

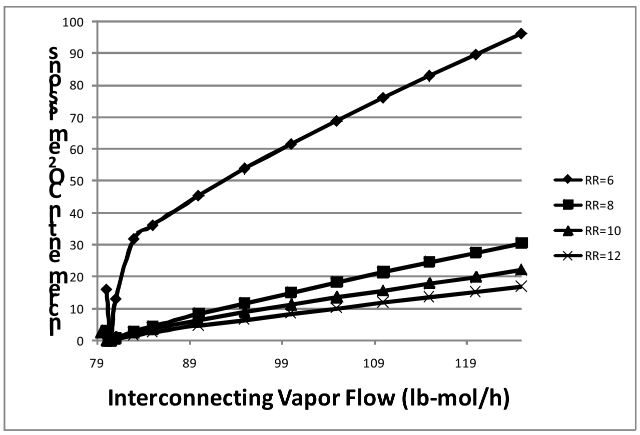


Figure 3 Increase in carbon dioxide emissions for different operational conditions in the thermally coupled distillation sequence with a side rectifier.

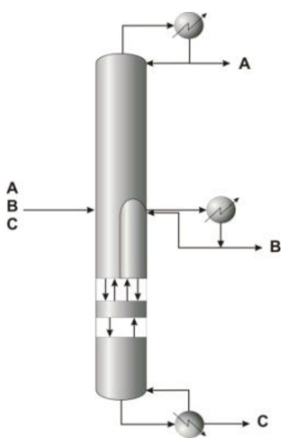


Figure 4. Practical implementation of the reactive TCDS with a side rectifier.

5. Conclusions

The esterification of methanol and lauric acid using sulphuric acid as catalyst was studied in a thermally coupled distillation sequence with a side column and the Petlyuk distillation column using a multi objective genetic algorithm with restrictions. The thermally coupled distillation sequence with a side rectifier was the best option in terms of energy consumption and purity of biodiesel in the product. The results for the reactive complex distillation sequence with a side column showed that energy consumption can be reduced drastically depending on operational conditions, and for conditions different than those of the optimal solution, carbon dioxide emissions can increase significantly. Finally, a practical implementation using a single column with a dividing wall is proposed.

6. Acknowledgements

We acknowledge the financial support provided by Universidad de Guanajuato, CONACyT and CONCyTEG (Mexico).

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