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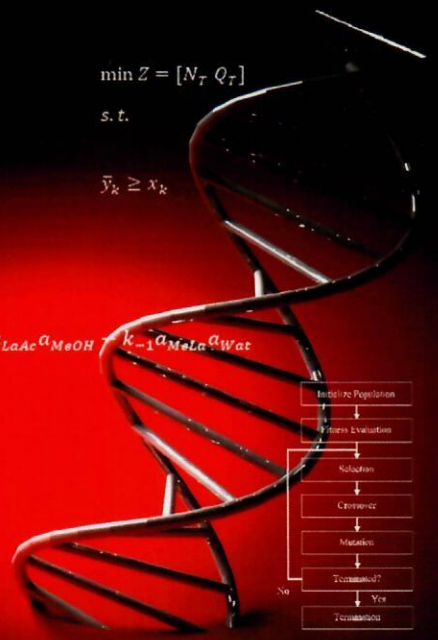

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GENETIC ALGORITHMS

ADVANCES IN RESEARCH AND APPLICATIONS

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EDITOR

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PREFACE

In Chapter One, a revision and complementary analysis of three interesting cases where stochastic strategies are applied to get the optimal design of intensified schemes is presented. The revisited cases include multicomponent, extractive and reactive thermally coupled distillation. Chapter Two performs parameter optimization on a genetic algorithm to skip the tuning parameter process during unmanned aerial vehicle path planning. Results show that truncation selection at 20% is highly recommended for genetic algorithm path planning application because of its low average path and computational costs. Chapter 3 describes the calibration of the numerical model of the Monte da Virgem telecommunications tower, located near the city of Porto, Portugal. The calibration of the numerical model of the tower relies on the application of an iterative method based on a genetic algorithm. Chapter 4 describes the genetic algorithm-based calibration procedure for a microscopic traffic simulation model, focusing on freeways and modern roundabouts. For both case studies, the genetic algorithm tool in MATLAB® was applied in order to reach the convergence between the outputs from Aimsun microscopic simulator and the observed data.

Chapter 1 - One of the main drawbacks of distillation relies on its high energy requirements. To reduce the total heat duty on separations with distillation, the use of thermally coupled distillation sequences has been proposed. Other enhanced distillation methods include extractive distillation and reactive distillation. All the aforementioned intensified distillation systems are modelled through a set of non-lineal equations. Thus, the optimization of the design of those complex distillation schemes is not an easy task, and robust optimization methods are required. Stochastic optimization methods have the capacity to deal with highly non-lineal, non-convex models with a high

number of decision variables. In this work, a revision and complementary analysis of three interesting cases where stochastic strategies are applied to get the optimal design of intensified schemes is presented. The revisited cases include multicomponent, extractive and reactive thermally coupled distillation. Optimal designs of these cases are generated with a stochastic optimization method, which is a multiobjective genetic algorithm with constraints handling. The optimization involves the simultaneous minimization of total heat duty, associated with operation cost, and the number of trays, which is directly related with the equipment cost. In order to comply with the desired recoveries and purities, inequality constraints are required; which are handled through a multiobjective approach, also avoiding solutions outside the feasible region. The columns are modelled in a rigorous way, since the algorithm is coupled to the process simulator Aspen Plus. Moreover, to enhance the convergence speed, neuronal networks are used as surrogate model; so the optimization can be performed in a faster way. Finally, an analysis of the results of the optimization procedure are presented, highlighting the implication for the production processes in terms of environmental impact and sustainability.

Chapter 2 - Genetic algorithm has been widely used in numerous fields, including in solving structural optimization problems, financial decision problems, and docking of flexible ligands, among others. Recently, researchers have developed significant interest in applying genetic algorithm in unmanned aerial vehicle path planning. Despite the advantages of genetic algorithm, several parameter inputs are required before using this algorithm. They include waypoint, population size, crossover rate, and mutation rate. The performance of this algorithm is dependent on these parameter settings. Thus, parameter optimization is performed on this algorithm to skip the tuning parameter process during unmanned aerial vehicle path planning. Results show that truncation selection at 20% is highly recommended for genetic algorithm path planning application because of its low average path and computational costs. In addition, a population size of 40 is suitable in unmanned aerial vehicle path planning. Last but not least, the optimum mutation rate of 10% is recommended based on the average path and computational cost for this algorithm.

Chapter 3 - This chapter describes the calibration of the numerical model of Monte da Virgem telecommunications tower, located near the city of Porto, Portugal. The tower is composed by a concrete shaft and a steel mast with a total height of 177 m. The calibration of the numerical model of the tower relies on the application of an iterative method based on a genetic algorithm. This method is based on the resolution of an optimization problem, which

involves the minimization of an objective function by varying a set of preselected model parameters. The objective function includes residuals associated to natural frequencies and mode shapes. The calibration results show a very good agreement between numerical and experimental modal responses and an improvement of the numerical model before calibration. Also the stability of several parameters, considering different initial populations, has proved the robustness of the genetic algorithm applied to the optimization of numerical models.

Chapter 4 - This chapter describes the genetic algorithm-based calibration procedure for a microscopic traffic simulation model, focusing on freeways and modern roundabouts. For both case studies, the genetic algorithm tool in MATLAB® was applied in order to reach the convergence between the outputs from Aimsun microscopic simulator and the observed data. The automatic interaction with Aimsun software was implemented through an original external Python script. Results showed that the genetic algorithm-based calibration procedure gave a better match to the observed data than simple manual calibration and the efficiency of the calibration efforts resulted significantly improved. At last, the calibrated model was applied to calculate the passenger car equivalents for heavy vehicles which represent the starting point for the operational analysis of roads and intersections.

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Chapter 1

GENETIC ALGORITHMS: A TOOL FOR OPTIMIZING INTENSIFIED DISTILLATION SEQUENCES

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ABSTRACT

One of the main drawbacks of distillation relies on its high energy requirements. To reduce the total heat duty on separations with distillation, the use of thermally coupled distillation sequences has been proposed. Other enhanced distillation methods include extractive distillation and reactive distillation. All the aforementioned intensified distillation systems are modelled through a set of non-lineal equations. Thus, the optimization of the design of those complex distillation schemes is not an easy task, and robust optimization methods are required. Stochastic optimization methods have the capacity to deal with

highly non-lineal, non-convex models with a high number of decision variables. In this work, a revision and complementary analysis of three interesting cases where stochastic strategies are applied to get the optimal design of intensified schemes is presented. The revisited cases include multicomponent, extractive and reactive thermally coupled distillation. Optimal designs of these cases are generated with a stochastic optimization method, which is a multiobjective genetic algorithm with constraints handling. The optimization involves the simultaneous minimization of total heat duty, associated with operation cost, and the number of trays, which is directly related with the equipment cost. In order to comply with the desired recoveries and purities, inequality constraints are required; which are handled through a multiobjective approach, also avoiding solutions outside the feasible region. The columns are modelled in a rigorous way, since the algorithm is coupled to the process simulator Aspen Plus. Moreover, to enhance the convergence speed, neuronal networks are used as surrogate model; so the optimization can be performed in a faster way. Finally, an analysis of the results of the optimization procedure are presented, highlighting the implication for the production processes in terms of environmental impact and sustainability.

INTRODUCTION

The separation of fluid mixtures is an important task in chemical and petrochemical industries. There are many applications on which it is necessary obtaining pure products from a mixture, or recovering reactants for its reuse on the process. One of the most used separation processes worldwide is distillation, which makes use of the difference on boiling points between the components of the mixture. Nevertheless, one of the main drawbacks of distillation relies on its high energy requirements, which is a consequence of its inherent low second-law efficiency. To reduce the total heat duty on separations with distillation, the use of thermally coupled distillation sequences has been proposed; and it has been reported that, for a given set of feed compositions of ternary mixtures, such sequences may reduce energy requirements in 30-50%, in comparison with a conventional distillation train [1, 2].

Although distillation is a well-known separation method, it cannot be used to obtain high purities of all the fluid mixtures. There are mixtures which must be separated using special methods, because its thermodynamic nature is highly non ideal or even with the presence of azeotropes. Thus, for such

mixtures it is usually not possible to reach high purities using conventional distillation. Some methods have been proposed to modify the volatilities between the components of the mixture, which involve using an external agent, such as in azeotropic distillation and extractive distillation [3]. Using those methods, high purities can be achieved for the components of the original mixtures. Nevertheless, additional separation is required to recover the solvent. Moreover, since the process still involves the mass and energy transfer inherent to distillation, energy requirements can still be high. In order to increase the thermodynamic efficiency of such processes, and reduce its energy requirements, the use of thermally coupled azeotropic and extractive distillation has been recently proposed [4-6].

Other enhanced distillation method implies carrying on reactions and separation in a single equipment; this intensified process is known as reactive distillation. Such schemes have several improvements if compared with the conventional sequence reactor-distillation column: the chemical equilibrium limitations can be override, the selectivity can be enhanced for multiple chemical reactions, energy requirements decrease when exothermic reactions occurs, and capital costs can also be reduced [7]. Nevertheless, since various phenomena are occurring simultaneously, the operative window is smaller than for the case of separated operations; i.e., the reactive and phase equilibrium must occur under the same conditions. Thermal coupling of reactive distillation systems has also been proposed, in order to reduce even more the energy requirements [8-10].

All the aforementioned intensified distillation systems (thermally coupled distillation, extractive distillation and reactive distillation) can be modelled through the well-known MESH equations [11], which consist on material balances, energy balances, sum constraints, and equilibrium equations. Component material balances involves bilinear terms, which causes non-convexity on the feasible region. Moreover, the thermodynamic models used to compute the equilibrium constants are highly non-linear, and the whole optimization problem usually involves several decision variables. Thus, the optimization of the design of those complex distillation schemes is not an easy task, and robust optimization methods are required. Recently, the interest on stochastic (meta-heuristic) strategies has increased, due to its capacity to deal with highly non-lineal, non-convex models with a high number of decision variables. In particular, the application of stochastic strategies to intensified schemes has been a very active research field; especially for cases where thermodynamic behavior is complex. Therefore, in this work a revision and complementary analysis of three interesting cases where stochastic strategies

are applied to get the optimal design of intensified schemes is presented. The revisited cases include multicomponent [12], extractive [5] and reactive [10] thermally coupled distillation. First, the application cases are presented. Then, the optimization tool and its main features are described, along with the formulation of the optimization problem for each case of study. Finally, an analysis of the results of the optimization procedure are presented, highlighting the implication for the production processes in terms of environmental impact and sustainability.

Case Studies

As a first case of study, the optimal design of thermally coupled distillation sequences for the separation of a multicomponent hydrocarbon stream is presented [12]. Three thermally coupled systems are studied: thermally coupled direct sequence (STAD, Figure 1.a), thermally coupled indirect sequence (STAI, Figure 1.b) and dividing wall column (DWC), which is represented by the thermodynamically equivalent Petlyuk column (Figure 1.c).

The sequences shown in Figure 1 are used to separate a multicomponent hydrocarbons mixture, whose flow rates, in kg/h, are listed next: n-propane to n-heptane (10.1255), n-octane to n-tetradecane (21.6061), n-pentadecane (0.2157), i-pentadecane (0.06901), n-hexadecane (0.2299), i-hexadecane (0.0736), n-heptadecane (19.0796), i-heptadecane (6.1055), n-octadecane (20.1919), i-octadecane (6.4614); being the total flow rate 84.1582 kg/h. These hydrocarbons are separated in three cuts: light gases (n-propane to n-heptane), biojet fuel (n-octane to i-hexadecane), and green diesel (n-heptadecane to n-octadecane). The recoveries of the key components are fixed in 99%. Phase equilibrium is modeled with the Chao-Seader correlation, since it is a reliable model for hydrocarbon mixtures.

The second case of study involves on the separation of a mixture of isopropanol (A) and water (B), with a molar feed composition of 0.5/0.5 [5]. An azeotrope exists for that binary mixture at a composition of 87%wt of component isopropanol, with a temperature of 80 °C [13]. In order to obtain high-purity of both components, dimethyl sulfoxide is used as solvent [14]. Thermodynamic behavior is modelled with UNIQUAC, which properly predicts the existence of the azeotrope [5].

Feed flow rate of solvent dimethyl sulfoxide is unknown, then it represents a degree of freedom of the system. Both, the mixture to be

separated and the solvent are introduced in a dividing wall extractive distillation column, as it is shown in Figure 2. Minimal recoveries and purities for each component are fixed as 99 mol%.

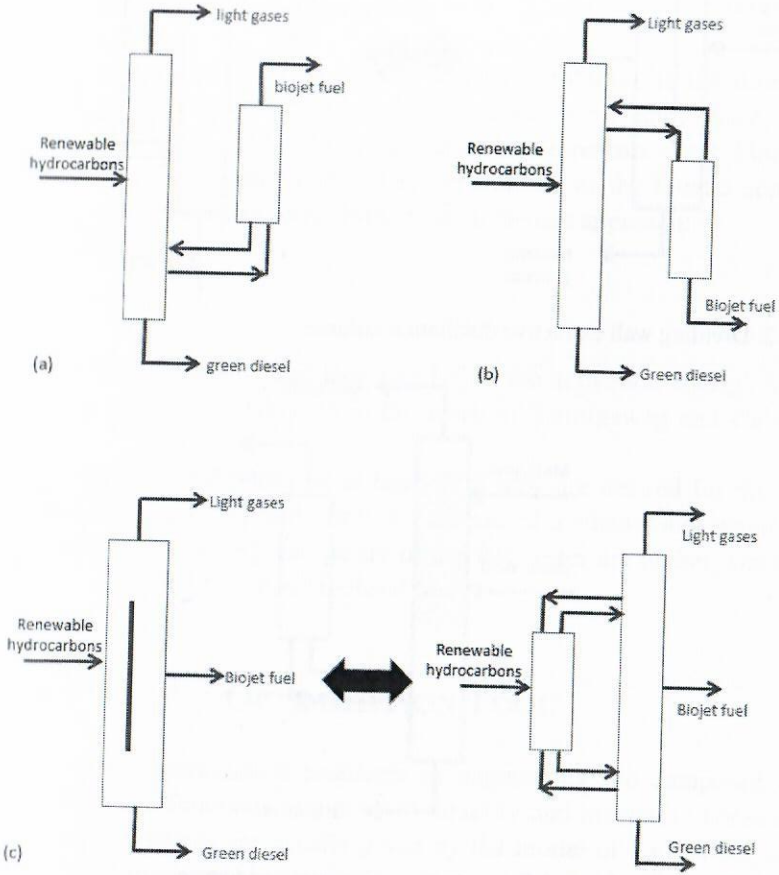

Figure 1. Thermally coupled distillation sequences: (a) thermally coupled direct sequence, TCDS, (b) thermally coupled indirect sequence, TCIS, (c) dividing wall column and Petlyuk column.

The third case of study involves performing the reaction between lauric acid and methanol to produce fatty ester and water [10]. Simultaneously, the product fatty ester requires to be purified; thus, the use of reactive distillation is proposed. Moreover, to reduce the energy requirements of the system, a thermally coupled direct reactive distillation sequence is used (Figure 3).

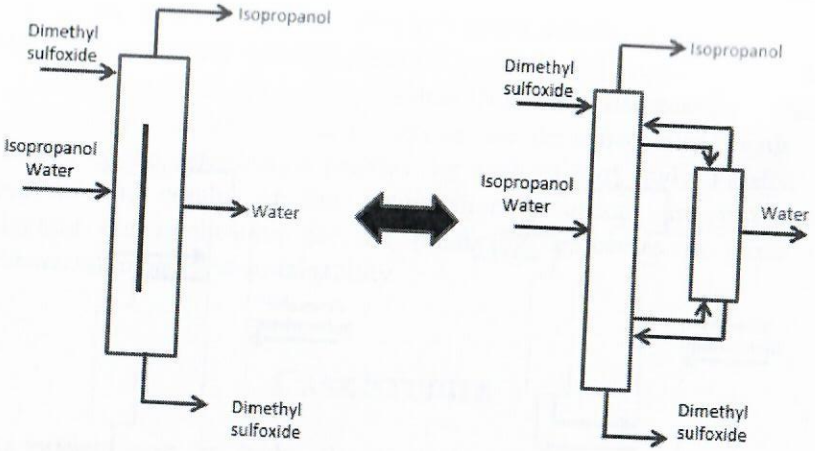

Figure 2. Dividing wall extractive distillation column.

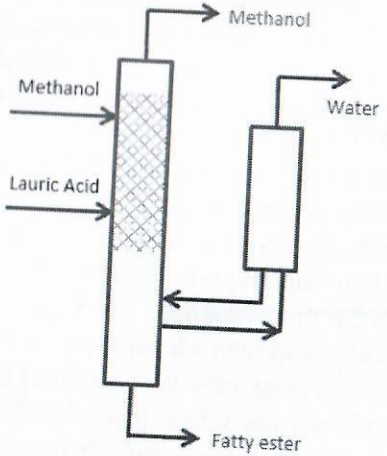

Figure 3. Thermally coupled direct reactive distillation sequence.

The reaction takes place as follows:

$$Methanol + Lauric\ acid \leftrightarrow Methyl\ laurate + Water \quad (1)$$

In this case, the reactants methanol and lauric acid are fed to the reactive direct thermally coupled distillation column (Figure 3) with a molar flowrate of 45.4 and 54.48 kmol/h, respectively. To represent the phase equilibrium, the UNIFAC thermodynamic model is used. The reaction can be modelled using

the pseudo-homogeneous kinetic model reported in Steinigeweg and Gmehling [15], assuming that the kinetics for the decanoic acid can be applied for the case of lauric acid. The kinetic model is, thus:

$$r = k_1 a_{LaAc} a_{MeOH} - k_{-1} a_{MeLa} a_{Wat} \quad (2)$$

In equation (2), k_1 and k_{-1} are the kinetic constants for the direct and reverse reactions, respectively, *LaAc* represents the lauric acid, *MeOH* stands for methanol, *MeLa* is the methyl laurate and *Wat* represents water. Finally, a_i is the activity of the component *i*. The dependence of the kinetic constants with temperature are represented through an Arrhenius approach:

$$k_j = A_j exp\left(\frac{-E_j}{RT}\right) \quad (3)$$

where A_j is the pre-exponential factor and E_j is the activation energy. Values for those parameters are taken from the work of Steinigeweg and Gmehling [15].

Here, recovery and purity of at least 99.9 wt% are desired for the ester, while the desired recovery and purity for unreacted methanol and water were fixed as 98%. The recovery and purity of the fatty ester are higher, since it is the required value for its use as biodiesel fuel.

Optimization Tool

Most of the optimization problems in engineering are composed by a vector of objective functions and a set of equality and inequality constraints. The equality constraints are usually given by the model of the system, while the inequality constraints rise from bounds for the variables. Some common objective functions involve maximizing a profit, minimizing costs, minimizing environmental impact, among others. In some cases, the optimization problem is simplified through the use of a single objective function. Nevertheless, a more reliable approach when looking for the best solution in engineering problems involves multiobjective optimization.

Stochastic, or meta-heuristic, optimization methods are a set of strategies which involves a directed search on the whole feasible region. This implies that such methods evaluates the objective function for different possible solutions, avoiding the necessity of computing derivatives. Moreover, the

methods can work even if there is not a model, and the only information available are input-output data. Among the meta-heuristic optimization methods, genetic algorithms have gained importance because of its capacity to find sets of optimal solutions. The method requires to be initialized with a set of randomly generated initial values, which is known as initial population; this represents a great difference with respect to mathematical programming techniques. The initial population is then evaluated to determine which of the individuals have the best characteristics (i.e., the best values for the objective functions), allowing them passing to the next generation (or iteration). Here, similarity can be observed with the natural evolution concepts. Once the population has been evaluated, the best individuals combine their genetic information between them and a new generation is obtained. This continuously occurs until a stop criteria is reached. A more detailed description of the basic genetic algorithm can be obtained from the work of Gen and Cheng [16].

The above described genetic algorithm is the basic one, which applies for unconstrained optimization with a single objective. In the case of a multiobjective optimization, the algorithm should find the set of optimal solutions known as Pareto front. For a minimization, a Pareto optimum can be defined as a point where there is not any feasible vector which can decrease the value of one of the objectives without increasing at the same time the value of other objective. If we define J as the feasible region, it can be stated that a given point $\bar{z}^* \in J$ is a Pareto minimum if for any $\bar{z} \in J$ it the following condition is satisfied:

$$\wedge_{n \in I}[f_n(\bar{z}) \geq f_n(\bar{z}^*)] \tag{4}$$

or, at least, there is some $n \in I$ for which:

$$f_n(\bar{z}) > f_n(\bar{z}^*) \tag{5}$$

where I is the set of objective functions to optimize. It is said that $\bar{z}$ dominates a solution $\bar{w}$ if $f(\bar{z}) < f(\bar{w})$, where W is a subspace of J and $\bar{w} \in W$. If there is not a solution $\bar{z}$ dominating $\bar{w}$ in the subspace W, then it is said that $\bar{w}$ is not dominated in W. The non-dominated solutions are Pareto optima, and the whole set of Pareto optima originates the Pareto front [17]. In this work, the Pareto front is obtained using the NSGA-II algorithm [18].

In order to take into account the constraints involved in engineering systems, particularly the inequality constraints, a strategy to handle the constraints is required. In this proposal, the concept of non-dominance is taken

as a basis [19]. In order to do this, the population is divided into sub-populations, using as a criterion the total number of satisfied constraints. Then, the individuals satisfying the n constraints are taken as the best ones, followed by those individuals satisfying n-1 constraints, and so on. Inside each sub-population, the individuals are ranked following the NSGA-II method. Nevertheless, an additional objective is taken into account, which consists on minimizing the degree of unsatisfied constraints. The dominance of each sub-population is computed as:

$$dominance\{Z_1, Z_2, min[0, (\overline{g_{k1}} - \overline{g_{k2}})]\} \tag{6}$$

where Z_1 and Z_2 are the objective functions in competence, and $\overline{g_{k1}}$ and $\overline{g_{k2}}$ are the terms in an inequality of the form $\overline{g_{k1}} \leq \overline{g_{k2}}$. The previously described strategy is employed to optimize the intensified sequences, taking into account the inequality constraints. An important aspect is that the columns are modelled in a rigorous way, since the algorithm is coupled to the process simulator Aspen Plus; which allows using the whole set of MESH equations along with a wide set of thermodynamic models to represent the phase equilibrium. Nevertheless, the evaluation of the multiobjective function in the process simulator takes a lot of time. To enhance the convergence speed neuronal networks are used, which represent a surrogate model to evaluate objectives and constraints. Therefore, the required time to calculate the objectives and constrains functions is reduced and the optimization can be performed in a faster way.

Optimization Problem Statement

The optimization problem for the thermally coupled distillation sequences can be stated as follows:

$$\begin{aligned} &\min Z = [N_T \; Q_T] \\ &\quad s.t. \\ &\bar{y}_k \geq x_k \end{aligned} \tag{7}$$

The two objective functions, N_T and Q_T, are the total number of stages and the total heat duty, and are both function of the reflux ratio for each column with a condenser, R_i, the number of stages for each column, N_i, the location of the interlinking streams in the main column, N_j, the location of the side stream

(if exists), N_s, the feed stage, N_F, the interlinking flow rates, F_j. The vector $\bar{y}_k$ represents the obtained purity for each component, while the vector x_k is the desired purity. Of course, the problem statement is completed with the equality constraints given by the model of the columns.

As a first approach, numerical values are supposed for the operational variables acting as degrees of freedom of the columns, i.e., the reflux ratio and the interlinking flowrates. The physical variables of the columns are obtained taking as a basis the conventional distillation sequences and rearranging the stages [20, 21]. Such initial systems are simulated in Aspen Plus, and the purities of the products are fixed at the minimal acceptable value using design specifications. Then, this initial design is used to generate the first population, which is sent to Aspen Plus in order to obtain values for objectives and constraints functions. The process continues until the maximum number of generation is reached.

In the case of the extractive distillation sequence, the objective function can be stated as in equation (7). Nevertheless, in this case N_T and Q_T are function of the reflux ratio for each column with a condenser, R_i, the number of stages for each column, N_i, the feed stage, N_F, the feed stage for the solvent, $N_{F,E}$, the solvent flow rate, F_E, and the interlinking flow rates, F_j. In order to obtain an initial design for the dividing wall extractive distillation sequence, numerical values are first supposed for the number of stages, the feed stages, the molar flow rate of the solvent and the interlinking flow rates; because there is not a shortcut method for the design of such system. The scheme is then simulated in Aspen Plus, using the initial guess for the required variables. The purity of the top and bottoms products in the main column are fixed with a design specification. Once having the initial design for the extractive distillation sequence, the initial population is randomly generated and the optimization procedure starts.

The objective function for the reactive distillation column is equal to that presented by the equation (7). For this system, N_T and Q_T are function of the reflux ratio for the reactive distillation column, R_i, the number of non-reactive stages, N_{NR}, the number of reactive stages, N_R, and the feed stages for each reactant, N_{F1} and N_{F2}. It is important to mention that since the unreacted methanol and fatty ester are fixed as constraints, indirectly the conversion is considered as an objective. There is not available a short-cut method for reactive distillation. Thus, the initial design of the reactive distillation column was obtained by guessing the number of reactive and non-reactive stages, and the location of the reactant streams. Such structure is simulated using Aspen Plus, manipulating the design if necessary, in order to increase the conversion

of the reactants and achieve the desired purities. Once it occurs, the purities are fixed through a design specification. Then, the initial population is generated taking as a basis the initial design and the optimization procedure starts.

RESULTS

In this section the analysis of the optimal designs of three intensified schemes for the previously described cases is presented. Also, the implications in terms of environmental impact and sustainability are discussed. It is important to recall that all the solutions on the Pareto front are optimal. Nevertheless, only one of them can be chosen, and this selection will depend on the particular necessities of the decision-maker.

For the case of multicomponent hydrocarbons mixture, the Figure 4 shows the Pareto front for the three thermally coupled systems analyzed, which are obtained using 1000 individuals and 90 generations. It can be observed that direct thermally coupled distillation sequence is the one with the lowest energy consumption, followed by the indirect sequence; the higher energy consumption is observed in the dividing wall column, which is indeed in another magnitude order. Therefore, for this mixture dividing wall distillation column is not the best option. An interesting aspect is related with the distribution of the stages in the intensified sequences. In the direct and indirect thermally coupled distillation sequences, the first column has a major number of stages, in the range of 70-130; while the second column has a small number of stages, under 40 for both sequences. In counterpart, the dividing wall column has a small number of stages in the first column, and a high number of stages in the second one. This can explain the significant difference in energy consumption between these schemes, even when the total number of stages can be similar.

With illustrative purposes, the characteristics of the designs with similar energy consumption are presented in Table 1. From Table 1, it can be seen that for a similar energy consumption the total number of stages in the schemes is different. The minor number of stages is found in the direct thermally coupled distillation sequence; the indirect thermally coupled distillation sequence has a major number of stages, even greater than the one of the dividing wall column. This observation exhibits the important role of adequate distribution of the stages in the energy consumption of the sequence. From these schemes the direct thermally coupled distillation sequence has the minor environmental

impact, and also the minor capital costs. Therefore, the purification of hydrocarbons with this sequence will help to having a more sustainable production process.

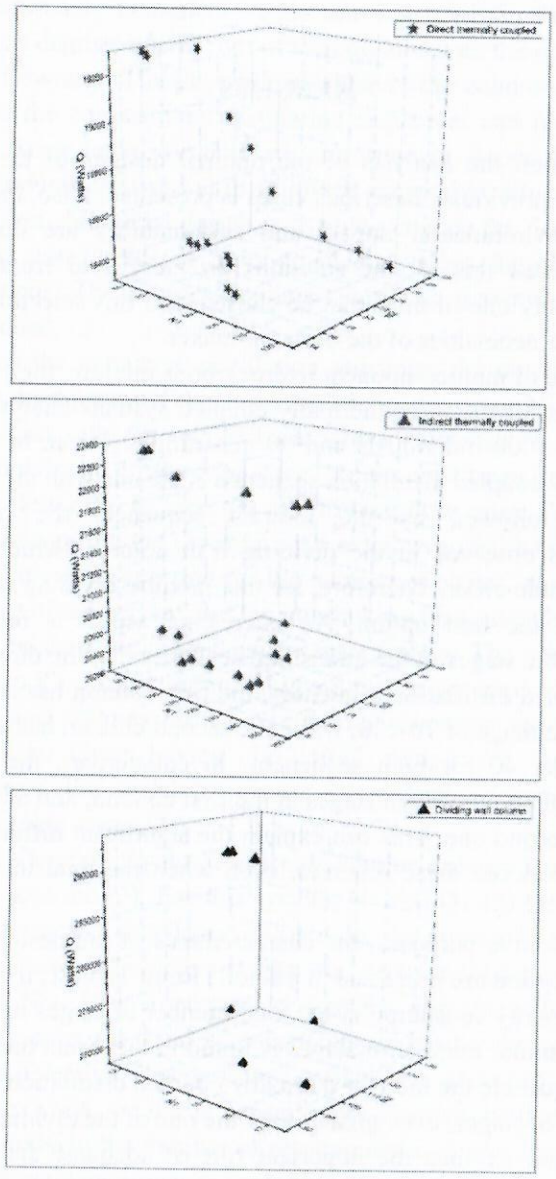

Figure 4. Pareto front for the thermally coupled distillation sequences.

Table 1. Selected designs from the Pareto front for the thermally coupled sequences

	Number of stages in first column	*Number of stages in second column*	*Heat duty, W*
Direct thermally coupled sequence	74	28	23,153.78
Indirect thermally coupled sequence	60	15	23,286.44
Dividing wall distillation column	14	140	269,458.09

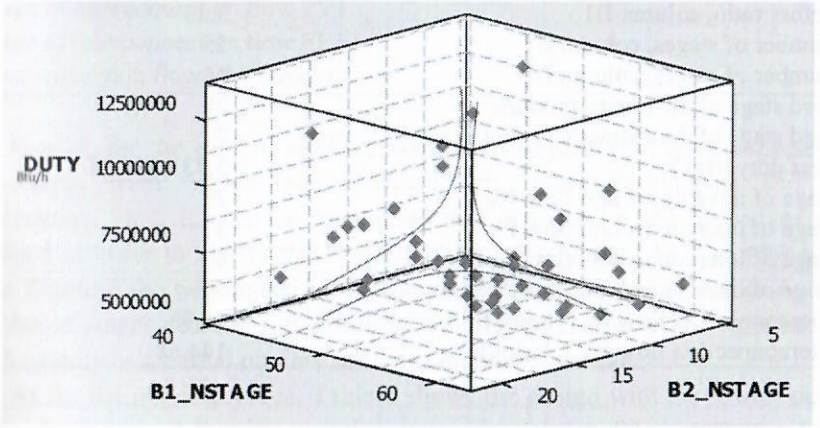

Figure 5. Pareto front for the dividing wall extractive distillation sequence.

For the case of extractive distillation sequences, the Pareto front includes the energy consumption and number of stages in both distillation columns, Figure 5; the front was obtained with 2500 individuals and 40 generations. It can be noticed that the minimum energy consumption depends on having a high number of stages in the first column, and an intermediate number of stage in the second one.

In Table 2, the design for the extractive dividing wall distillation column with minimum energy consumption is showed. From Table 2, it can be observed that the extractive agent is not fed to the column in the second stage as usually occurs, but in stage 7. Also, the configuration that presents the minimum energy consumption has four different interconnection stages, instead of the traditional two. Moreover, we can observe that the interconnection flows are small. Therefore, they are not increased as

consequence of the use of an extractive agent. This result is quite interesting since the thermally coupled distillation sequences are a feasible option to perform extractive separations, finding that the interconnection flows are not increased due to the extractive agent. This implies an environmental friendly process, which allows obtaining products through a sustainable production process.

Table 2. Design for the extractive dividing wall distillation column with minimum energy consumption

Design variable	Value
Reflux ratio, column B1	3.13
Number of stages, column B1	55
Number of stages, column B2	14
Feed stage of the binary mixture	28
Feed stage of the extractive agent	7
Heat duty, Btu/h	5,733,134.64
Stage of interconnection flow FV1	29
Stage of interconnection flow FV2	37
Stage of interconnection flow FL1	4
Stage of interconnection flow FL2	51
Interconnection flow FL1, kmol/h	77.93
Interconnection flow FV2, kmol/h	144.68

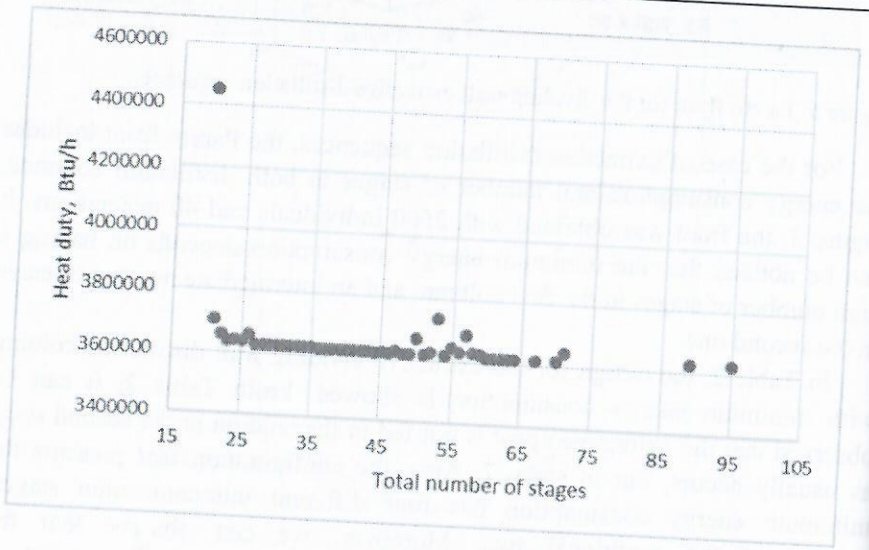

Figure 6. Pareto front for the thermally coupled direct reactive distillation sequence.

Table 3. Design for the thermally coupled direct reactive distillation column with minimum energy consumption

Design variable	Value
Reflux ratio, column B1	0.046
Number of stages, column B1	62
Number of stages, column B2	8
Reactive stages, column B1	32
Feed stage of lauric acid	4
Feed stage of methanol	32
Heat duty, W	1,059,726.84
Stage of interconnection flow FV1	12
Stage of interconnection flow FL1	4
Interconnection flow FL1, kmol/h	19.37

Finally, for the case of reactive distillation sequences, Figure 6 presents the Pareto front, which was obtained using 2000 individuals and 40 generations. First, it must be mentioned that in Figure 6 the objectives are grouped in order to clarify the visualization of the results. As it can be seen from Figure 6 the two objectives in competition are clearly presented. As the number of stages decreases, the heat duty increases. However, the variation of the heat duty as the total number of stages increases is small.

As for the previous cases, Table 3 shows the design with the lowest duty. It can be observed that the reactive stages in column B1 represent a high percentage of the total number of stages, with pure physical purification is performed mainly in the second distillation column. Also, we can observe that the interconnection flows are small, in comparison with the fed streams to the reactive sequence. Moreover, the reflux ratio are also small, and as consequence the heat duty of the sequence is low.

In this case, the production of methyl laurate was studied using a reactive thermally coupled distillation scheme. The intensification is feasible and reduced operational and capital costs are expected. Due to the reduction in heat duty, this process is environmental friendly and sustainable.

CONCLUSION

A compilation and complementary analysis of the optimal design of thermally coupled distillation sequences with a stochastic, multiobjective

evolutionary strategy was presented. Since the optimization tool is coupled to the Aspen Plus process simulator, all the results are obtained considering the complete material and energy balances along with the rigorous phase equilibrium models. The strategy has been shown to be robust for the design of complex systems, as thermally coupled, extractive and reactive sequences, which are modelled by highly non-convex equations and have a high number of degrees of freedom. The robustness of the method for extractive and reactive systems is quite important, since nowadays shortcut methodologies for this kind of systems are scarce or limited in its application to simple cases. Also, this strategy allows obtaining optimal designs, which are environmental friendly. This tools is of great value nowadays where the development of sustainable biomass conversion processes is required.

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