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Process Alternatives for Biobutanol Purification: Design and Optimization

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ABSTRACT: Biobutanol is primarily used as a solvent or component in surface coatings. It has characteristics similar to petroleum fuel and is considered as a superior biofuel to ethanol. Biobutanol is more energy dense and less hygroscopic than ethanol, resulting in higher possible blending ratios with gasoline. Development of technologies for biobutanol production by fermentation has resulted in higher final biobutanol concentrations, less fermentation byproducts, and higher volumetric productivities during fermentation, together with less energy intensive separation and purification techniques. These new technological developments have the potential to provide a production process for biobutanol that is economically viable in comparison to the petrochemical pathway for its production. In this study, we have analyzed and compared four different possible process designs for the purification of biobutanol production. Process modeling in Aspen Plus was performed, and the optimization was conducted using a differential evolution algorithm. Our results indicated that the process consisted of a liquid−liquid equilibrium (LLE) column followed by steam stripping distillation proved to be a profitable design in current economic conditions, which was evaluated trough total annual cost (TAC) calculation. This alternative process can be employed on an industrial scale to improve the process economics of biobutanol production.

1. INTRODUCTION

With the current reduction of petroleum resources and considering the amounts of fuel used in transportation which have direct impact in environmental concerns, such as climate change, depleting fossil fuel reserves, and reducing reliance on imports, the use of biofuels for transport is becoming very relevant.[1] Some reports indicate that transport could be responsible of 28% of total U.S. greenhouse gas emissions (near to 2000 t of CO_2), this represents a huge impact just below of the electricity sector, also trends reported indicate an increase about 18% since 1990.[2] Attending to these needs, the renewable fuel standard program (RFS) was created by the United States Environmental Protection Agency; this program established the first renewable volume mandate. The RFS program required 7.5 billion gallons of renewable fuel to be blended into gasoline by 2012, and it will be increased by 36 billion gallons in 2022.[3] Thus, several current research projects are leading to identifying new methods, technologies, or routes in order to increase the potential of renewable energy sources to substitute current fuel transportation demands, a good alternative for this could be biobutanol.

Biobutanol is a fuel that can be obtained from renewable sources, such as rice straw, corn fiber, and so on, further using Clostridium acetobutylicum or Clostridium beijerinckii either hexoses and pentoses, contrary to traditional production of ethanol, where only hexoses can be utilized. Biobutanol from renewable sources has some interesting thermodynamic properties that other fermentation-derived products do not have. The average energy density of biobutanol represents 30% more than ethanol, closer to gasoline, moreover biobutanol's vapor pressure facilitates its applications, and it is less soluble to water, has a lower volatility, and can be blended with gasoline in any proportion.[4] Biobutanol produced by fermentation (acetone butanol ethanol (ABE) or AB) is a very old fermentation process employed for commercial production, its production was discovered by Pasteur in 1861. However, currently, the major production of butanol proceeds from petroleum sources by the oxo process.[5] In recent decades, big efforts were made in genetic studies in some Clostridium species used in ABE fermentation, with focus on improved fermentation characteristics. Nevertheless, the major hurdles making this kind of biological process profitable are the high cost of the substrate, the low solvent concentration in fermentation broth, and finally the high product recovery and purification cost as analyzed by Van der Merwe et al.[6] On the basis of these developments, it is expected that biobutanol could help in several factors such as instability of oil supplies from the Middle East, a readily available supply of renewable agricultural-based biomass, and the reduction of greenhouse gas emissions.[6] Traditionally, ABE fermentation is carried out in a batch reactor, and after that, product is purified using distillation. Despite ABE fermentation having been studied by several researchers, the concentration of biobutanol in broth is pretty low because of toxicity problems. Additionally other components, such as ethanol and acetone are produced, which

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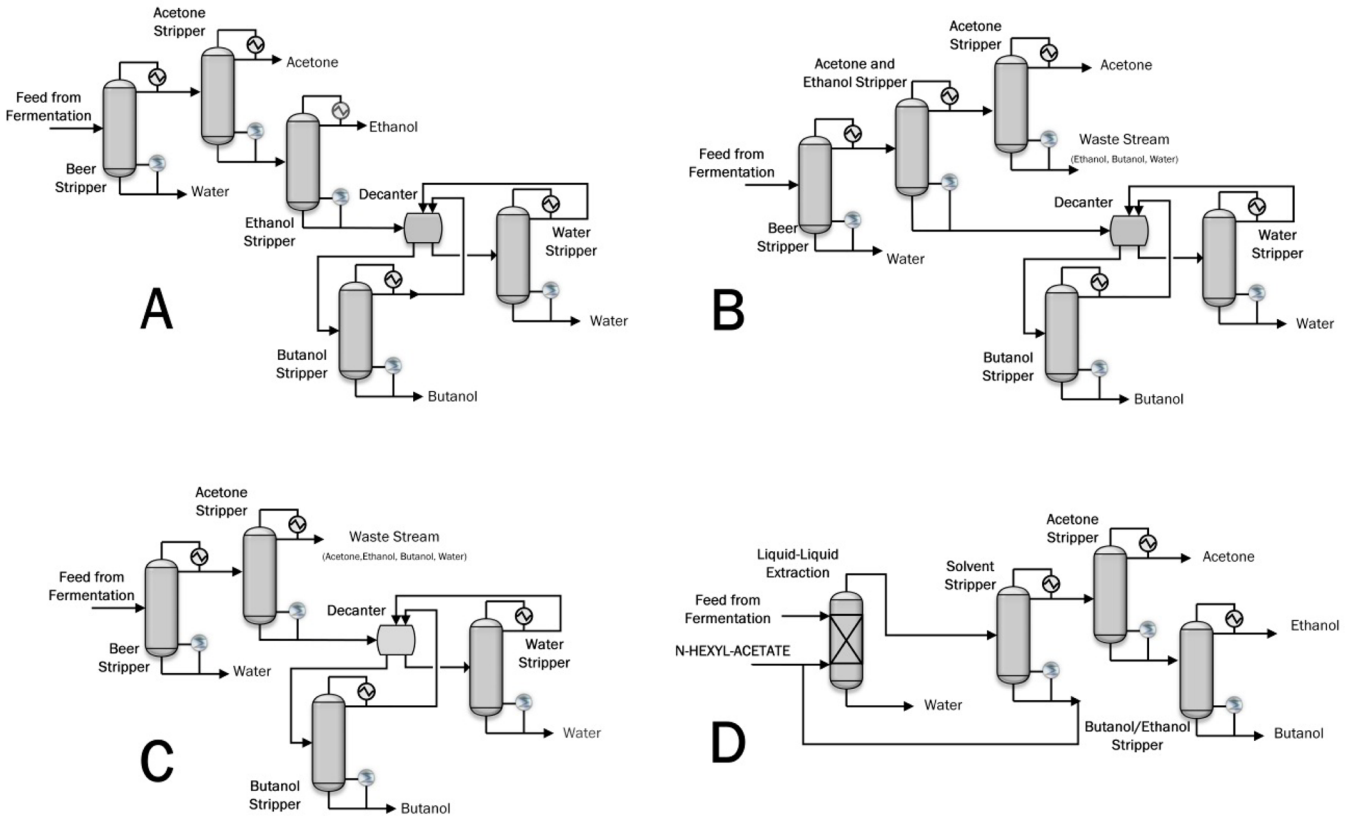

Figure 1. Processes studied in the recovery of biobutanol.

ought to be removed or purified from the same broth coming from the fermenter.[7]

Limited attention has been paid to the distillation process in the production of acetone/biobutanol and its optimization. Distillation processes are well-studied technologies, and despite the energy consumption and efficiency in purification, it is expected that optimization applied to distillation based separation technologies combined with efforts in genetic modification of strain involved in fermentation, could influence greatly reducing water and increasing biobutanol concentration in broth fermentation and would lead ABE fermentation to a more sustainable place compared with traditional petroleum fuels.[8]

The aim of this work is to perform the process design, optimization, and comparison of four different possible process routes for industrial scale biobutanol production from agricultural crops and molasses. Process route A, B, and C consisted of steam stripping distillation and distillation columns, while in Process D some of the distillation columns were replaced with a liquid−liquid extraction column (see Figure 1). Process modeling in Aspen Plus was performed, and the optimization was conducted using the stochastic optimization method differential evolution with a tabu list.[9] These four process routes have been synthesized previously by Van der Merwe et al;[6] however they did not apply a formal optimization strategy for the development of these process designs. In fact, applying a rigorous optimization strategy, several effects of each freedom degree involved in these designs can be watched; in this manner, it is possible to identify some optimal alternatives which can open the opportunity to new intensified designs, expecting an improvement in economic indicators, or in a wider point of view could be considered environmental issues. Results of this study are useful to evaluate an alternative process that can be employed on an industrial scale in light of a global optimization strategy.

2. PROBLEM STATEMENT

Product recovery represents a big challenge associated with the production of biobutanol on an industrial scale due to the low concentration obtained from fermentation broth, which can lead to great energy consumption during separation and purification processes. Recovery techniques should show term stability, high selectivity, and a considerable removal rate.[10] The purification process is also complicated due to the formation of a homogeneous azeotrope between ethanol and water and a heterogeneous azeotrope between biobutanol and water.

Recently, Van der Merwe et al.[6] reported four alternatives to purify all the components from ABE fermentation (Figure 1). These process routes employed technology similar to previous industrial processes for biobutanol production, and all these process are fed of a fermentation broth from a batch fermentation followed by distillation columns to purify components. For this work, process route A (Figure 1) was defined using the base case process design simulated in the study by Roffler et al.[11] where all components from ABE fermentation are purified. This process design also includes a decanter to perform the heterogeneous azeotrope separation. Process route B (Figure 1) is also based on the process design reported by Roffler et al.[11] This process design is equally fed from a fermentation broth; however, the third distillation column does not purified ethanol such as Process route A does. Instead of that, the ethanol flow is totally mixed with wastewater and biobutanol traces. Process route C (Figure 1) was defined using the process design studied by Marlatt and

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Datta.[12] In this design, only biobutanol flow is purified, and both ethanol and acetone leaving the purification process are mixed with water and biobutanol traces. Finally, process route D (Figure 1) is slightly different than process routes A, B, and C, since first distillation column is replaced with a liquid−liquid extraction column, using hexyl acetate as extractant agent, in order to separate both homogeneous and heterogeneous azeotropes. After that three distillation columns perform the separation of acetone, biobutanol, and ethanol.

In this study, all these design cases were initially simulated using Aspen Plus process models. Note that these process models were robust and thermodynamically rigorous. According to Van der Merwe et al.[6] and Chapeaux et al.,[13] NRTL-HOC was the most accurate thermodynamic model for the calculation of the physical property available for the components used at the specified conditions. Note that it was assumed that all process designs have the same stream feeds except LLE design where it was added hexyl acetate as extractant.

3. OPTIMIZATION PROBLEM

The optimized operation of the biobutanol fermentation processes is essential to run a biobutanol industry that can compete effectively with the current biobutanol derived from the petrochemical route, once the acetone, biobutanol, and ethanol (ABE) fermentation, as normally is called the fermentation to produce biobutanol, is characterized by its low productivity.

Next, the optimization problem is established for each process sequence, considering the objectives, constraints, and design variables involved. Overall, all design problems are formulated as a constrained global optimization problem.

3.1. Process Route A and B. In process designs A and B, the objective function is the minimization of the total annual cost (TAC), which is directly proportional to the heat duty, services, and column size. The minimization of this objective is subject to the required recoveries and purities in each product stream, i.e.:

$$\begin{aligned} &\text{Min(TAC)} = f(N_{tn}, N_{fn}, R_{rn}, F_{rn}, D_{cn}) \\ &\quad \text{subject to } \vec{y}_m \geq \vec{x}_m \end{aligned} \tag{1}$$

where N_{tn} are total column stages, N_{fn} is the feed stages in column, R_{rn} is the reflux ratio, F_{rn} is the distillate fluxes, D_{cn} is the column diameter, y_m and x_m are vectors of obtained and required purities for the m components, respectively. This minimization implies the manipulation of 25 continuous and discrete variables for each route process, where 5 variables are used for the design of each column. Note that since the product streams flows are manipulated, the recoveries of the key components in each product stream must be included as a restriction for the optimization problem. In route process A, the acetone, biobutanol, and ethanol must be recovered; while in route process B, the acetone and biobutanol must be recovered.

3.2. Process Route C. This process route has also one objective function. The minimization of this objective is subject to the required recoveries and purities in each product stream and the optimization problem is defined as

$$\begin{aligned} &\text{Min(TAC)} = f(N_{tn}, N_{fn}, R_{rn}, F_{rn}, D_{cn}) \\ &\quad \text{subject to } \vec{y}_m \geq \vec{x}_m \end{aligned} \tag{2}$$

This optimization problem implies the manipulation of 20 decision variables for each route process. Note that the difference between this route and routes A and B is the purities in acetone and ethanol product streams and the recovery of the same components.

3.3. Process Route D. This route has also the same objective function. Nevertheless, since first distillation column is replaced with a liquid−liquid extraction column, the number of decision variables is reduced in that column, where the stages of column and feed stage are just optimized. The optimization problem is defined as

$$\begin{aligned} &\text{Min(TAC)} = f(N_{tn}, N_{fn}, R_{rn}, F_{rn}, D_{cn}) \\ &\quad \text{subject to } \vec{y}_m \geq \vec{x}_m \end{aligned} \tag{3}$$

Overall, 17 decision variables are considered in the design of this route process, where 2 design variables are related to the liquid−liquid extraction column. All design variables for the cases of study are described in Table 1.

Table 1. Decision Variables Used in the Global Optimization of Process Routes for Biobutanol Production

	Process route A	Process route B	Process route C	Process route D
number of stages C1	×	×	×	×
number of stages C2	×	×	×	×
number of stages C3	×	×	×	×
number of stages C4	×	×	×	×
number of stages C5	×	×		
feed stages C1	×	×	×	×
feed stages C2	×	×	×	×
feed stages C3	×	×	×	×
feed stages C4	×	×	×	×
feed stages C5	×	×		
reflux ratio C1	×	×	×	
reflux ratio C2	×	×	×	×
reflux ratio C3	×	×	×	×
reflux ratio C4	×	×	×	×
reflux ratio C5	×	×		
distillate rate C1	×	×	×	
distillate rate C2	×	×	×	×
distillate rate C3	×	×	×	×
distillate rate C4	×	×	×	×
distillate rate C5	×	×		
diameter C1	×	×	×	×
diameter C2	×	×	×	×
diameter C3	×	×	×	×
diameter C4	×	×	×	×
diameter C5	×	×		
total	**25**	**25**	**20**	**17**

4. GLOBAL STOCHASTIC OPTIMIZATION STRATEGY

Particularly, the optimization and design of processes routes are highly nonlinear and multivariable problems, with the presence of both continuous and discontinuous design variables; also, the objective functions used as optimization criterion are potentially nonconvex with the possible presence of local optimums and subject to constraints.

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Table 2. Results of the Global Optimization of TAC for the Process Routes A and B

	Process route A					Process route B				
	C1	C2	C3	C4	C5	C1	C2	C3	C4	C5
Column Topology										
number of stages	7	35	41	12	8	5	25	21	5	4
feed stage	4	30	20	2	6	4	13	13	3	2
Specifications										
distillate rates (lbmol/h)	1.58	1.732	1.714	0.618	0.676	2.037	0.318	0.285	0.575	0.520
reflux ratio	1.602	18.731	64.943	12.645	2.567	0.082	5.624	5.167	0.638	1.031
diameter (ft)	1.049	1.784	1.150	1.600	2.013	1.032	1.003	0.997	0.997	1.014
Solvent Feed Streams										
acetone flow rate (lb/h)	16.9502					16.9502				
butanol flow rate (lb/h)	30.1808					30.1808				
ethanol flow rate (lb/h)	0.7289					0.7289				
hexyl acetate flow rate (lb/h)	0					0				
Product Streams										
acetona putiry (wt %)		0.9957						0.9988		
butanol purity (wt %)					0.9996				0.9951	
ethanol purity (wt %)			0.949					0.7770		
Energy Requirements										
reboiler duty (cal/s)	105621	75776	20506	155445	61680	46195	28517	22381	22389	24010
condenser duty (cal/s)	−93707	−74968	−20480	−152222	−58414	−39614	−27311	−22410	−17022	−19080
economic evaluation										
capital cost ($)	28786	55139	45082	36473	36762	26052	29143	28462	27241	25674
total annual cost ($/y)			256696					155020		

Table 3. Results of the Global Optimization of TAC for the Process Routes C and D

	Process route C				Process route D			
	C1	C2	C3	C4	LLE	C1	C2	C3
Column Topology								
number of stages	7	37	22	14	4	24	35	31
feed stage	6	35	14	10	2	13	29	19
Specifications								
distillate rates (lbmol/h)	1.587	1.619	0.825	0.835		0.715	0.293	0.015
reflux ratio	6.341	14.817	11.849	0.547		0.902	6.903	15.031
diameter (ft)	1.008	1.084	1.170	1.421	0.9978	0.942	0.944	0.943
Solvent Feed Streams								
acetone flow rate (lb/h)	16.9502				16.9502			
butanol flow rate (lb/h)	30.1808				30.1808			
ethanol flow rate (lb/h)	0.7289				0.7289			
hexyl acetate flow rate (lb/h)	0				2013.1			
Product Streams								
acetona putiry (wt %)		0.8383					0.9983	
butanol purity (wt %)				0.9997				0.9990
ethanol purity (wt %)			0.0360					0.9960
Energey Requirements								
reboiler duty (cal/s)	197721	23384	9646	34884		280971	30771	4162
condenser duty (cal/s)	−185808	−22892	−7211	−31639		−24796	−29617	−4066
Economic Evaluation								
capital cost ($)	19305	34868	28393	32253	2336	30200	32395	30008
total annual cost ($/y)		149020				136827		

Then, in order to optimize the processes routes for biobutanol production, we used a stochastic optimization method, differential evolution with tabu list (DETL).[9] Differential evolution (DE) has its basis in Darwin's natural selection theory and is similar to genetic algorithms (GAs) except for one important factor: several GAs, particularly earlier versions, encode decision variables as bit strings whereas DE encodes them as floating-point numbers. Srinivas and Rangaiah[9] showed that the use of some concepts of the metaheuristic tabu can improve the performance of DE algorithm. In particular, the tabu list (TL) can be used to avoid the revisit of search space by keeping record of recently visited points, which can avoid unnecessary function evaluations. Based on this fact, Srinivas and Rangaiah[9] proposed the hybrid method DETL, which includes classical DE steps, TL, and tabu check to keep track of the evaluated points for avoiding revisits to them during the optimization search, and a convergence criterion based on

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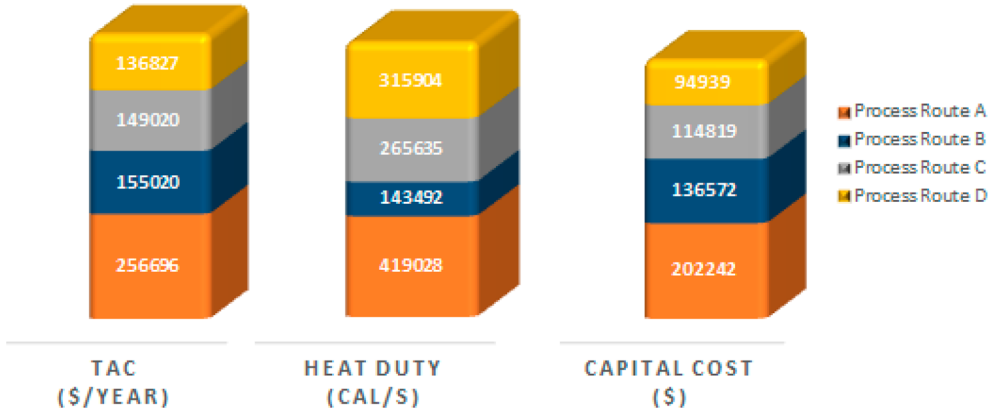

Figure 2. Comparative values of optimization results.

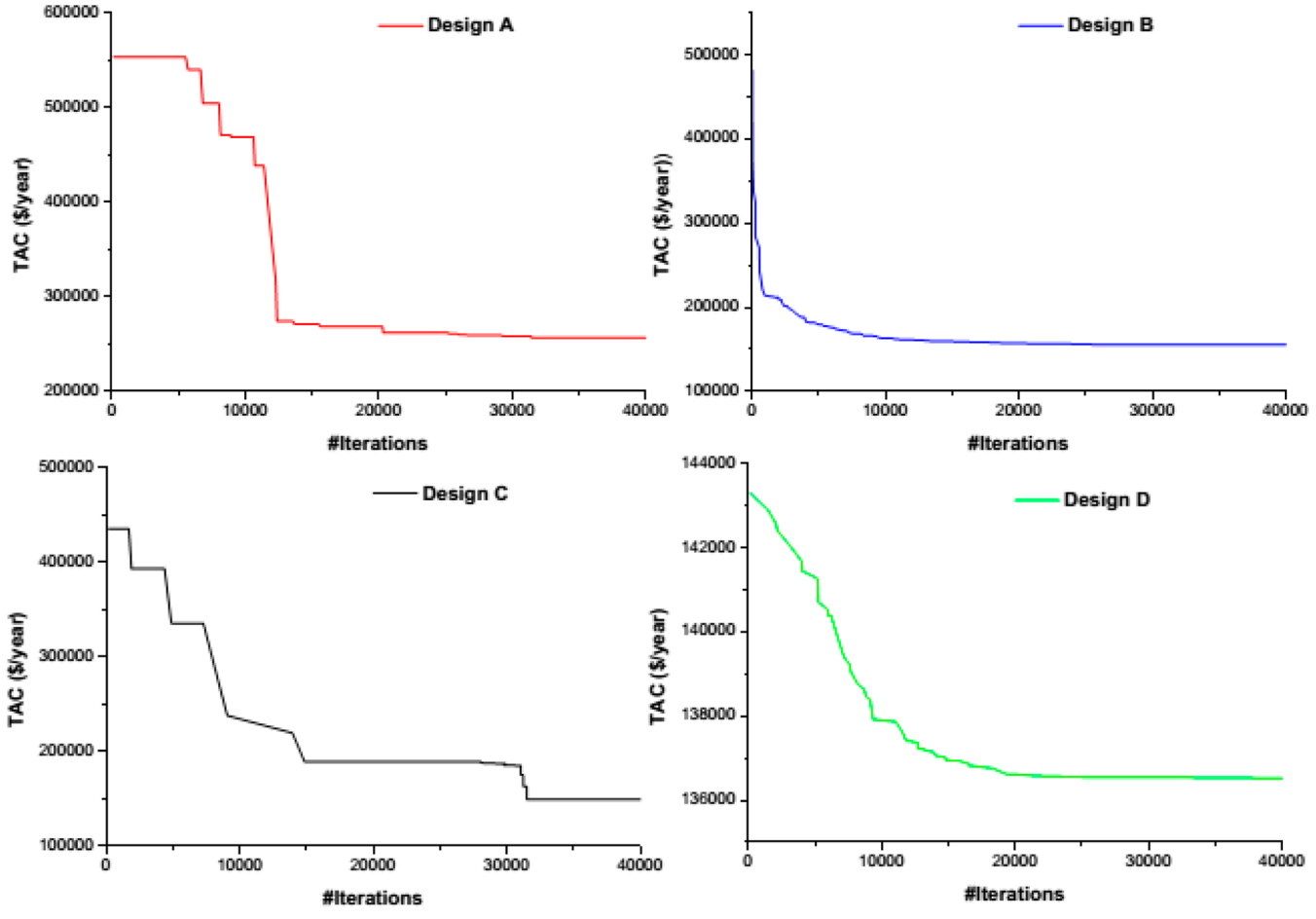

Figure 3. Optimization results of process configurations A, B, C, and D for the recovery of biobutanol.

maximum number of generations. A comprehensive description of this DETL algorithm is provided by Srinivas and Rangaiah.[9]

The implementation of this optimization approach was made using a hybrid platform using Microsoft Excel and Aspen Plus. The vector of decision variables (i.e., the design variables) are sent to Microsoft Excel to Aspen Plus using DDE (dynamic data exchange) through COM technology. In Microsoft Excel, these values are attributed to the process variables that Aspen Plus need. After simulation it is done, Aspen Plus return to Microsoft Excel the resulting vector. Finally, Microsoft Excel analyzes the values of the objective function and proposes new values of decision variables according to the stochastic optimization method used. For the optimization of process routes analyzed in this study, we have used the following parameters for DETL method: 200 individuals, 300 generations, a tabu list of 50% of total individuals, a tabu radius of 0.000 002 5, 0.80, and 0.6 for crossover and mutation fractions, respectively. These parameters were obtained through a tuning process via preliminary calculations. The tuning process consists of performing several runs with different number of individuals and generations, in order to detect the best parameters that allow obtaining the better convergence performance of DETL.

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In order to calculate the total annual cost (TAC) used as the objective function, we used the method published by Guthrie,[14] which was modified by Ulrich.[15] It performs cost estimation of an industrial plant separated in units, and using equations published by Turton et al.,[16] we carried out a cost approximation of the process using eq 4, i.e.:

$$\mathrm{TAC} = \frac{\sum_{i=1}^{n} C_{\mathrm{TM},i}}{n} + \sum_{j=1}^{n} C_{\mathrm{ut},j} \tag{4}$$

Where TAC is the total annual cost, C_{TM} is the capital cost of the plant, n is the total number of individual units, and C_{ut} is the cost of services, respectively.

5. ANALYSIS OF RESULTS

In this section, we present the results for all process routes where the total annual cost was evaluated as the objective function. It is important to recall that all results presented are designs that satisfy each restriction of purity, i.e., biobutanol 99.5% (wt %), acetone 98% (wt %), and ethanol 95% (wt %) for process route A; biobutanol 99.5% (wt %) and acetone 98% for process route B; biobutanol 99.5% (wt %) for process route C; biobutanol 99.5% (wt %), acetone 98% (wt %), and ethanol 99% (wt %) for process route D; and at least 95% (wt %) recovery of ethanol, 99% (wt %) recovery of acetone and biobutanol, and 99.9%(wt %) hexyl acetate recovery, respectively.

Before the optimization process and using an average feed stream,[17] see Table 2 and 3, all sequences were modeled and simulated rigorously in Aspen Plus V7.2 using the RadFrac module. This means that all designs presented were obtained considering the complete set of MESH (mass balances, equilibrium relationships, summation constraints, energy balance) equations along with the phase equilibrium calculations.

5.1. Optimization Results. Through the optimization process were obtained several points for all four process routes which accomplish all purities and recovery restriction; however at the end of this process, we could get a single point which represented the smallest economic impact measured by TAC. In order to differentiate each process, some process results must be analyzed such as heat duty, capital cost and total annual cost, Figure 2 shows in a general way how Process route A spends a relative big heat duty compared with the other three process routes; likewise, this happens with capital cost, the best point obtained of Process route A generates a bigger economic impact compared again with the other process. This behavior is clearly due to the fact that acetone, ethanol, and biobutanol are purified using only distillation columns.

5.2. Behavior of the Objective Function. Evaluating TAC as an objective function, Figure 3 shows the convergence behavior of TAC in the process optimization. Despite this, we have performed more function evaluations in our calculations, the optimization results are presented until 40 000 evaluations because the vector of the decision variables does not produce a significant improvement. Under this scenario, it was assumed that DETL achieved convergence at the tested numerical conditions and the reported results correspond to the best solution obtained by the DETL method.

After the optimization process, Process route A showed a final value of $256,696, Process route B showed a final value of $155,020, Process route C showed a final value of $149,020 and, finally, Process route D showed a final value of $136,826. Results reported by Van der Merwe et al.[6] show that Process route D has the smallest heat duty between the four processes, which is consistent with the results obtained in the present study, and it is expected that this process route has the lowest carbon emissions too. Similarly, they concluded that Process route C has the smallest heat duty between Process designs A, B, and C, which again is totally consistent with the result presented here; also, Process route C has the smallest cost among all four process design. It is convenient to remark that Van der Merwe et al.[6] did not apply a formal optimization strategy for the development of their process designs. Then, comparing TAC from Process routes A, B, and C, which involved only distillation columns, it is observed that purifying ethanol in route A represents nearly 41% more TAC compared with Process route C, further purifying acetone and ethanol in route B represents 39% more compared with Process route A.

Table 2 shows the general characteristics of process routes A and B, and Table 3 shows the corresponding optimized design variables for process routes C and D. As it can be seen, in the first column of sequences A, B, and C, where water is preferably split, the optimization method converged at designs with few stages, which impacts directly in a minor costs. However, the next steps in the purification of the ABE components require bigger distillation columns and a great amount of heat duty. Despite the fact that process route D turned out to have more stages among process designs B and C, it can be seen that its design does have the smallest heat duty of the designs, which generates a large reduction in its TAC. On the contrary, process routes A, B, and C need more energy to purify all components, and the big difference, which produces a bigger TAC of these process routes, comes directly from capital cost, which is affected by the geometry of distillation columns (vessel, reboiler, condenser, etc.). This effect produces bigger capital cost, compared to process design D. On the other hand, despite the fact that process route B has the least amount of stages due to only acetone and biobutanol being purified and its heat duty is slightly bigger than process route D, the total annual cost generated is bigger. In addition, the capital cost of this process route is bigger than process route D, which produces obviously a bigger TAC. Process route C, where only biobutanol is purified, uses a smaller amount of energy in comparison to process route A which produces again a smaller capital cost than process route A. Process route D, especially analyzing the results reported in Table 2 for distillation columns C1, C2, and C3, requires relatively little energy to do its separations. However, the size of those columns is bigger than those obtained for process routes A, B, and C. Moreover Figures 4 and 5 show the composition and temperature profiles obtained in Process route D.

Also, Tables 2 and 3 shows that Processes A, B, and C, having larger costs than Process route D, have quite different operational variables among them. Due to the fact that Process route D can separate homogeneous and heterogeneous substances in a liquid−liquid column, the next stages use columns with relatively smaller reflux ratios. On the other hand, Process routes A, B, and C imply designs that handle relatively high values of reflux ratios.

Furthermore, considering that Process route D showed the best economic indicator measured by TAC, it is possible to improve its performances including a hypothetical thermal coupling among all three distillations involved in ABE purification, which can generate some thermodynamically equivalent sequences as shown in Figure 6. Moreover, a side

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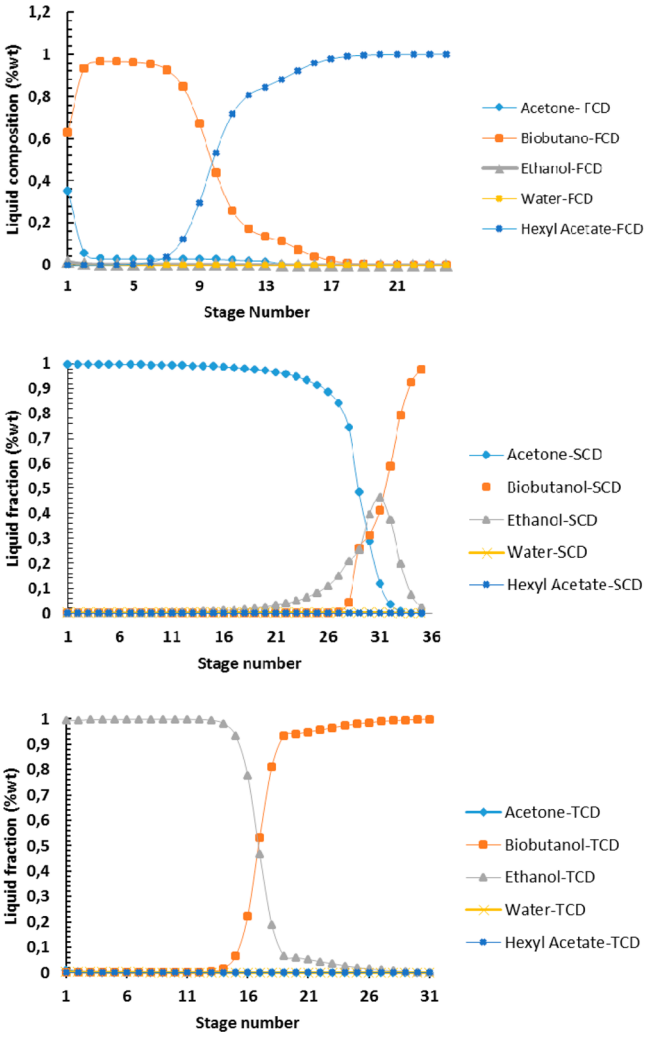

Figure 4. Composition profiles for each distillation column in Process route D.

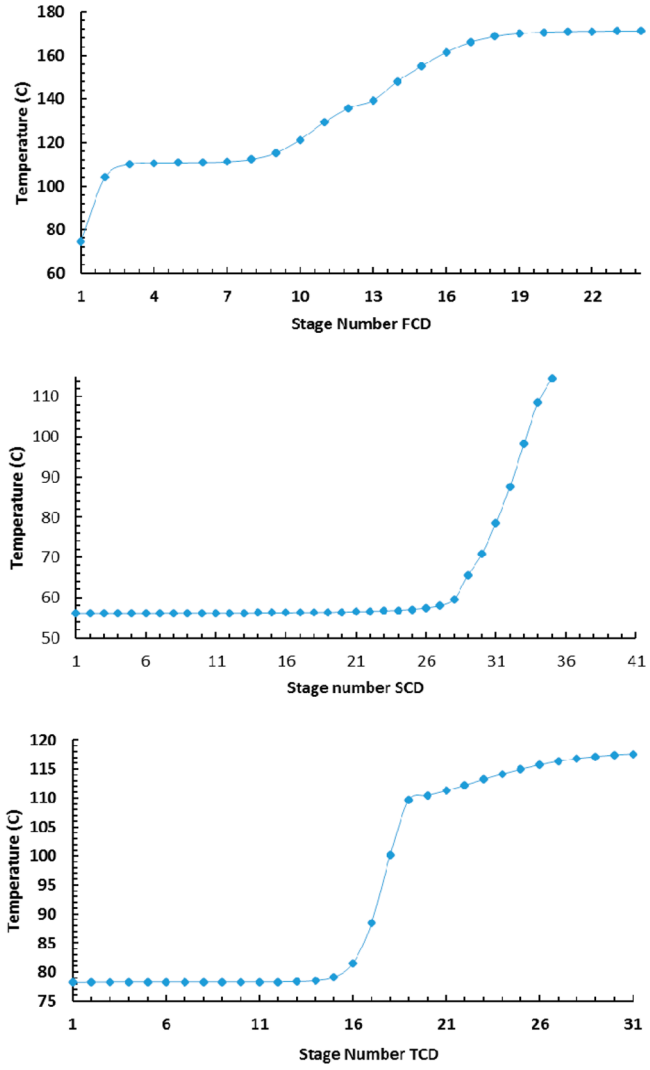

Figure 5. Temperature profiles for each distillation column in Process route D.

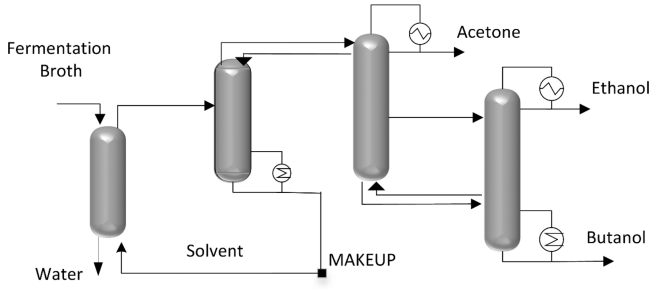

Figure 6. Thermally coupled sequence for ABE purification.

stream could be introduced and the corresponding column section can be eliminated expecting energy and costs savings. The preliminary optimization problem is defined as

$$\text{Min(TAC)} = f(N_{tn}, N_{fn}, R_{rn}, F_{rn}, F_{vn}, F_{ln}D_{cn})$$
$$\text{subject to } \vec{y}_m \geq \vec{x}_m \quad (4)$$

Where new freedom degrees such as F_{ln} (liquid flow in interconnections) and F_{vn} (vapor flow in interconnections) are introduced at coupled sequences. This has shown that this sequence could reduce its TAC nearly 20% in similarly conditions compared with Process route D, opening opportunities for intensified designs that could show very interesting energy savings, operational cost savings, and probably industrial application.

5. CONCLUSIONS

In this study, we have applied a stochastic global optimization method for the process design of several routes for biobutanol production to improve their cost and performance. According to our results, Process route D showed the smallest TAC, with little difference with respect to Process route C. Process route A, where all components are purified, showed the biggest TAC due to capital cost of equipment and heat duty performing ABE purification. The optimized design processes imply small columns, whose design is preferable with few stages to reduce cost. Nevertheless, it would be interesting to determine the dynamic behavior of these designs in order to identify all their process advantages and disadvantages. Otherwise, this kind of research effort combined with results of other studies could lead in future years to a profitable ABE fermentation process, which could compete with traditional ways to produce biobutanol.

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Notes

The authors declare no competing financial interest.

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NOMENCLATURE

LLE = liquid−liquid extraction
TAC = total annual cost
ABE = acetone−butanol−ethanol
RFS = renewable fuel standard program
N_{tn} = total column stages
N_{fn} = feed stages
R_{rn} = reflux ratio
F_{rn} = distillate fluxes
D_{cn} = column diameter
y_m = vectors of obtained purities
x_m = vectors of required purities
DETL = differential evolution with tabu list
DE = differential evolution
Gas = genetic algorithms
TL = tabu list
DDE = dynamic data exchange
C_{TM} = capital cost of the plant
C_{ut} = cost of services
FCD = first distillation column of Process route D
SCD = second distillation column of Process route D
TCD = third distillation column of Process route D
F_{ln} = vapor flow in interconnections
F_{vn} = vapor flow in interconnections

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