Separation and Purification Technology 185 (2017) 149–159

Contents lists available at ScienceDirect

Separation and Purification Technology

journal homepage: www.elsevier.com/locate/seppur

Optimal hybrid separations for intensified downstream processing of biobutanol

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ARTICLE INFO

Article history:
Received 7 January 2017
Received in revised form 26 April 2017
Accepted 5 May 2017
Available online 20 May 2017

Keywords:
Biobutanol
Dividing wall column
Multi-objective optimization
Condition number

ABSTRACT

Current research focuses on new energy alternatives which could compete with the traditional energy sources based on fossil fuels, and eventually diminish the consequences on climate. Recently, butanol produced by ABE fermentation attracted more attention since its energy power is comparable to that of gasoline. But some hurdles are involved in the establishment of this fuel as an immediate substitute of fossil fuels, e.g. lower butanol concentration in the fermentation effluents and the expensive separation steps to purify the effluent.

This work is the first to report the use of hybrid separation based on liquid-liquid extraction (LLX) combined with dividing-wall column (DWC) technology for the purification of the ABE (acetone-butanol-ethanol) mixture. The configurations proposed are the result of multi-objective optimization that aims to find designs that fulfill the tradeoff between those objectives: cost minimization, reduce environmental impact, and increase controllability.

The downstream processing alternatives are designed and optimized by minimizing three objective functions simultaneously: the total annual cost (TAC) as an economical index, the eco-indicator 99 as an environmental function, and the condition number (CN) as control index. Among the four designs, the scheme where only a reboiler is included showed the best economic performances and relatively good values of condition number and eco indicator 99.

1. Introduction

Liquid biofuels obtained by biomass fermentation have attracted much attention because of their environmental-friendly origin. Although bioethanol enjoys currently mature knowledge, butanol is considered nowadays a promising liquid biofuel due to its properties such as higher energy content and lower volatility (as compared to ethanol), high flash point to ensure safe handling and transportation, and the possibility of blending it with gasoline in any percentage without any engine modification [1]. Fermentation of lignocellulosic material as substrate to produce butanol with the use of Clostridium strains seems assertive since such material can be obtained from agricultural residues [2,3]. During the past two decades, both experimental and computational engineering tried to enhance the performance of the ABE fermentation. Those attempts consider the development of new strains to upgrade product yield (due to the butanol inhibition of Clostridium strains), and new downstream processing alternatives that improve the efficiency of separation and purification [4]. The main drawback of fermentation processes is the production of diluted effluents that require energy intensive separation and purifications steps, which account for 60–80% of the total costs of the process [5].

In this respect, a combination of a decanter (exploiting the liquid phase split) or liquid-liquid extraction (LLX) combined with advanced distillation technologies, could be used to increase the concentration of the diluted stream and then purify the main product [5,6]. Other separation techniques that could be used include adsorption, gas stripping, vacuum flash, reverse osmosis (RO), perstraction, and pervaporation. But most of these technologies are still in the research and development phase, while LLX and distillation are proven already in biorefineries. Among the distillation technologies, diving wall column (DWC) is a promising alternative to separate and purify effluents produced by fermentation [7]. Owing to its high thermodynamic efficiency, DWC is a great example of heat-integrated distillation columns with many industrial applications [8–10].

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http://dx.doi.org/10.1016/j.seppur.2017.05.011
1383-5866/

Nomenclature

ABE	acetone-butanol-ethanol	MINLP	mixed integer nonlinear programming
LLX	liquid-liquid extraction	SVD	singular value decomposition
RO	reverse osmosis	VBA	Visual Basic
DWC	dividing-wall column	DDE	Dynamic Data Exchange
C_{TM}	capital cost	σ	singular values
C_{UT}	Cost of Services	Σ	Diagonal Matrix
TAC	total annual cost	γ	condition number
LCA	Life Cycle Assessment	U	Direction of the Process Outputs
CN	condition number	V	Direction of the Process Inputs
DE	differential evolution	TL	Taboo List
DETL	Differential Evolution with Tabu List	TS	Taboo Search
EI99	eco-indicator 99		

However, the optimal design of any kind of thermally coupled systems for multi-component separation is a non-linear and potentially non-convex problem [11]. Nonetheless, optimization techniques have shown key capabilities to improve several processes. In particular, stochastic optimization algorithms proved to be able to handle this kind of complex problems, since it is not necessary to have explicit data of the model or its derivatives [12]. Many previous studies focused on reducing the economic impact of separation processes [13], and the inclusion of more objectives has been considered from a multi-objective optimization point of view [14]. However, the control properties are not considered in a first design stage, as control issues are addressed and solved in a separate and sequential procedure. This design-then-control methodology may present some drawbacks, such as infringement of dynamic restrictions, over-design and low performance, so a global performance of any proposed design cannot be guaranteed [15]. The dynamic consequences lead to separation alternatives that would not be flexible on operative performance. In this manner, the variation of product specification and raw materials demands an appropriate control strategy able to address those issues. Under this scenario, a solution strategy requires the inclusion of several goals evaluated at the same time. This strategy must be capable of handling economic and environmental issues, along with integrating a process control strategy already at the design stage.

The idea of integrating design and control is not actually new, several authors have proposed to assess the dynamic properties with some index-based methods [16–18]. Those optimization strategies considered several ideas. For example, Luyben et al. [19] considered the dynamic control performance in the form of matrix norms or dynamically calculated error, this framework being solved as a mixed-integer optimal control problem. Seferlis and Grievink [20] developed an optimization strategy based on economic index and static controllability. Nevertheless, those controllability indexes were treated as constraints of the mathematical optimization problem or considered in the economic objective function through the weighted functions. Recently, Vazquez-Castillo et al. [21] proposed the inclusion of the condition number (CN) of the relative gain matrix in an operative nominal point, as control index to measure the natural dynamic properties of distillation columns. This control index allowed the evaluation of the dynamic properties considering a full and rigorous model of a separation process. Moreover, CN is a proper index to assess qualitatively the control properties of any design in steady-state. This index has been used in chemical processes for achieving such purpose [17,22]. It is therefore clearly necessary to propose a general method to evaluate simultaneously those economic, environmental and control capabilities of any proposed design.

This work is the first to propose several novel downstream processing schemes for the ABE fermentation, based on a combination of liquid-liquid extraction and dividing wall column. These new hybrid alternatives (LLX + DWC) were designed and evaluated under a robust optimization process by means of a hybrid optimization algorithm – Differential Evolution with Taboo List (DETL) – considering three simultaneous objective functions, the total annual cost (TAC), the eco-indicator 99, and the condition number as economic, environmental and controllability indexes, respectively. This optimization methodology allows including at early stage design conflicting objective functions trying to obtain process designs that are cheaper, environmentally friendly, and with good dynamic properties designs.

2. Problem statement

Two major problems are associated with butanol fermentation (ABE process): 1. very low concentration and yield owing to the severe butanol toxicity to microorganisms, which results in a dilute product and large disposal loads, and 2. high energy-demand recovery of butanol from the dilute fermentation broth. In this respect, enhancing the production of biobutanol would consist of two strategies: (1) a biological approach (engineering Clostridias metabolic pathways for butanol hyper-production), and (2) optimization of more efficient separation processes [23] (such as the ones described in the present study). Suitable process designs need to increase the yield of products, minimize the energy consumption and environmental impact.

To solve the problem of expensive downstream processing in the ABE fermentation, this study proposes a multi-objective optimization approach using three objective functions evaluated simultaneously: the total annual cost (TAC), eco-indicator 99, and the condition number as the economic, environmental impact and controllability indicators, respectively. However, there is a lack of strategies concerning the inclusion (at early design stages) of environmental, economic and controllability indexes that guarantee eco-efficient designs with good controllability properties. The enforcement of a multi-objective optimization approach provides a wider picture of the process performance, the role of all the design variables, and the objective functions evaluated here.

3. Case-study description

Recently Rong and Turunen [24] proposed a set of intensified DWC for quaternary mixtures, while Vazquez-Castillo et al. [25] evaluated those designs under a robust optimization strategy considering a quite complete set of mixtures considering a wide range of relative volatility differences and feed composition. Their results highlighted some designs which exhibited promising results concerning the economic evaluation. Moreover Sánchez-Ramírez et al. [13] reported that the inclusion of a liquid-liquid extraction column improves the separation of an ABE effluent since the extracting agent is able to separate two azeotropes, homogeneous (ethanol/water) and heterogeneous (butanol/water).

This study considers several hybrid designs combining a liquid-liquid extraction column (using hexyl-acetate as mass separating agent) and dividing wall columns, similar to those reported by Vazquez-Castillo et al. [25] but evaluated under a multi-objective optimization strategy using economic, environmental and controllability indexes respectively (see Fig. 1). In brief we take advantage of simultaneous thermal coupling and heat integration as a process intensification strategy to synthesize this separation process schemes. First, the number of condensers and reboilers are reduced introducing a thermal coupling in the streams of 'no-products' streams. This produces the heat-integrated thermally coupled configurations. Then, the prefractionation column without a stream with pure product in the heat-integrated thermally coupled configurations is incorporated into another column with dividing-wall. This produces the intensified new distillation systems with a reduced number of columns than heat-integrated thermally coupled configurations [20]. All these design cases were simulated by robust and thermodynamically rigorous Aspen Plus process models. According to Van der Merwe et al. [26] and Chapeaux et al. [27], the NRTL-HOC thermodynamic model was the most accurate for calculating the physical properties of the components used, at the specified conditions. All the binary interaction parameters related to the property model are available in the pure components databank of the Aspen Plus process simulator. This was validated against experimental data by Patrascu et al. [6].

Moreover, it was assumed that all process designs have the same illustrative feed stream, as previously reported by Wu et al. [28] (see Table 1), and hexyl-acetate was added as extractive agent. The product purities specified in all processes are: biobutanol >99.5 wt%, acetone >98 wt% and ethanol >95 wt% and over 98 wt % recovery of ethanol, 99 wt% recovery of acetone and biobutanol, and 99.9 wt% hexyl-acetate recovery, respectively.

4. Optimization indexes and formulation

This section describes the optimization indexes and the multi-objective optimization problem. The optimal conditions to operate the downstream processing of the effluent from ABE fermentation are of utmost importance to operate a competitive butanol biorefinery. Those optimal conditions must take into account several factors highlighting the economic and environmental performance, but the integration of a control index leads to a large scale optimization problem. The condition number was selected as controllability index considering that it has been already used in the control properties of downstream processes [22,29,30]

4.1. Total annual cost calculation

The total annual cost (TAC) was selected as index that measures the economic impact. To calculate the TAC, the method reported by Guthrie [31] and further modified by Ulrich [32] was used. This method estimates the cost of an industrial plant by means of equations published by Turton et al. [33]. The cost approximation of the process was carried using Eq. (1):

$$TAC = \frac{Capital\ costs}{Payback\ period} + Operating\ costs \tag{1}$$

Where the capital cost of the plant is calculated as the sum of the capital cost of all units $\sum_{i=1}^{n} C_{TM,i}$, and the operating cost as the sum of all the cost services $\sum_{j=1}^{n} C_{ut,j}$. A payback period of 3 years was used. Economic analysts often assume that the longer it takes to recover funds, the more uncertain are the positive returns. For this reason, they sometimes view payback period as a measure of risk, or at least a risk-related criterion to meet before spending funds. A company might decide, for instance, to undertake no major expenditures that do not pay for themselves in, in example, 3 years [34]. The plant is assumed to run 8500 h/year. Also, the following costs for heating and cooling were taken into

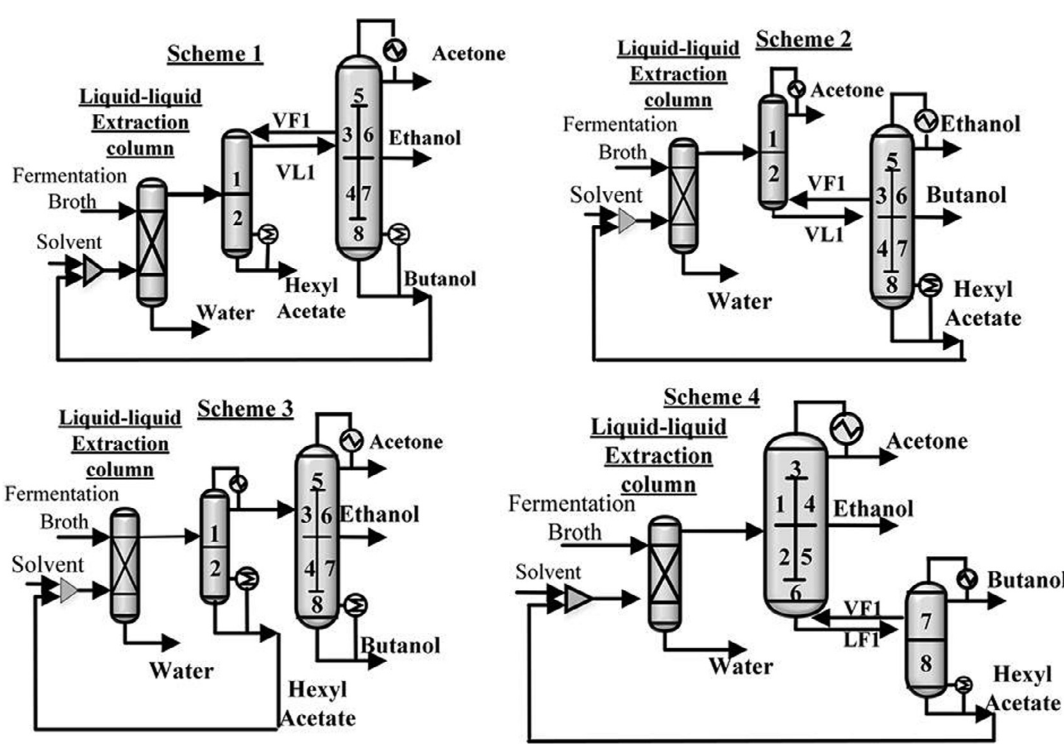

Fig. 1. Analyzed schemes for biobutanol purification.

Table 1
Feed characterization for the biobutanol purification process (Wu et al. [28]).

	Composition (mol%)	Composition (wt%)	Temperature (K)	322
Acetone	0.1128	0.1695	Vapor fraction	0
Biobutanol	0.0808	0.3018	Flow rate (kg·h^{-1})	45.3592
Ethanol	0.0043	0.0073		
Water	0.80198	0.5214		

account: high-pressure steam (42 bar, 254 °C, $9.88/GJ), medium-pressure steam (11 bar, 184 °C, $8.22/GJ), low-pressure steam (6 bar, 160 °C, $7.78/GJ) and cooling water (0.72/GJ) [35].

4.2. Environmental impact calculation

The environmental impact was quantified using the Life Cycle Assessment (LCA) principles by means of the eco-indicator 99 (EI99) [36]. This approach allows solving the eco-issues considering that the overall environmental impact is globally minimized. The eco-indicator 99 is calculated as follow:

$$EI99 = \sum_b \sum_d \sum_{k \in K} \delta_d \omega_d \beta_b \alpha_{b,k} \tag{2}$$

Where β_b represents the total amount of chemical b released per unit of reference flow due to direct emissions, $\alpha_{b,k}$ is the damage caused in category k per unit of chemical b released to the environment, ω_d is a weighting factor for damage in category d, and δ_d is the normalization factor for damage of category d. In the eco-indicator 99 methodology, 11 impact categories are considered [36] aggregated into three major damages categories: human health, ecosystem quality, and resources depletion. In this work, for eco-indicator 99 calculation the impact of three factors were considered as most important in the ABE downstream processing: steam (used in column reboiler), electricity (used for pumping) and steel (to build distillation columns and accessories). The values for those three factors are summarized in Table 2.

4.3. Controllability index calculation

The condition number is used as index to evaluate the controllability properties. Calculation of the condition number was carried out by means of the singular value decomposition (SVD) of the relative gain matrix of the evaluated design at nominal point. In other words, when a design accomplishes all restrictions, the singular values are obtained before calculating the condition number. The SVD is a numerical algorithm developed to minimize computational error involving in large matrix operations [37]. The singular value decomposition of a matrix (K in example) outcome in three component matrices according to the next equation [38]:

Table 2
Unit eco-indicator used to measure the eco-indicator 99 in both case studies (Geodkoop and Spriensma [36]).

Impact category	Steel (points/kg)	Steam (points/kg)	Electricity (points/kWh)
Carcinogenics	6.320E-03	1.180E-04	4.360E-04
Climate change	1.310E-02	1.600E-03	3.610E-06
Ionising radiation	4.510E-04	1.130E-03	8.240E-04
Ozone depletion	4.550E-06	2.100E-06	1.210E-04
Respiratory effects	8.010E-02	7.870E-07	1.350E-06
Acidification	2.710E-03	1.210E-02	2.810E-04
Ecotoxicity	7.450E-02	2.800E-03	1.670E-04
Land Occupation	3.730E-03	8.580E-05	4.680E-04
Fossil fuels	5.930E-02	1.250E-02	1.200E-03
Mineral extraction	7.420E-02	8.820E-06	5.7EE-6

$$K = U \Sigma V^T \tag{3}$$

Where: K is an $n \times m$ matrix, U is an $n \times n$ orthonormal matrix called the "left singular vector", V is an $m \times m$ diagonal of scalers called the "singular values" and are organized as follow: $\sigma_1 > \sigma_2 > \sigma_3 \ldots \sigma_m > 0$. Note in terms of matrix operations both U and V consists in a simple coordinate rotation. In matrix operation, the SVD calculates the rank and condition of a matrix and maps geometrically the strengths and weaknesses of a set of equation [37].

The attractive and interesting point of the SVD in terms of controllability is that when applied to a matrix which describes the steady-state aspect of multivariable process, the singular vectors and singular values have a very particular physic interpretation described as follows [37]: K the steady-state gain matrix represents the physically scaled steady-state sensitivity of each process sensor to change in each of the manipulated variable. U, the left singular vectors supplies the most accurate coordinate system for viewing the process sensors. In other words this coordinate system is such that the first singular vector $U1$ indicates the easiest direction in which the system must be changed, while $U2$ is the next easiest direction and so on. V the right singular vector indicates the most accurate coordinate system for viewing the manipulated variables, in such way is possible to know the combination of control actions which probably will has the most effect on the system. Σ as the diagonal of the singular values, supplies the ideal decoupled gain of the open loop process. The ratio between the largest singular to the smallest value is the condition number of the gain matrix and is a direct measure of the difficulty of the decoupled multivariable control problem [38].

The condition number is the ratio between the largest and the smallest singular value and is used to measure the "condition" of a set of equations.

$$\gamma = \sigma_{max} / \sigma_{min} \tag{4}$$

In terms of controllability, a large condition number indicates that it will be inconvenient to satisfy the entire set of control objectives (notwithstanding the control strategy to be used) [37]. Physically the condition number represents the ratio of the maximum and minimum open-loop, decoupled gains of the system. A large condition number suggests that the relative sensitivity of a system in one multivariable direction is very poor [37].

In this work, the condition number of the relative gain matrix is obtained in an open-loop control policy, each process design generates a relative gain matrix in a nominal state. The elements of each matrix are calculated considering a disturbance in the manipulated variable (reflux ratio, reboiler heat duty, side stream flowrate and so on). The magnitude of that perturbation was set as a 0.5% positive change in the values of those manipulated variables on its nominal state. The impact of these perturbations is sufficiently low that a first order response after perturbation can be assumed. It is remarkable that the relative gain matrix is scaled to consider changes of different order of magnitude in perturbation.

A disadvantage of using the SVD technique is the dependence of the system units used, since the SVD calculation will include the effect of such units. For example, in this study we consider three control variables, the mass purity of acetone, butanol and ethanol, these variable are limited between 0 and 1. However, we also used three manipulated variable, reflux ratio, bottoms flow rate and side stream flow rate [37,39]. To eliminate this disadvantage, in this work we propose to limit the manipulated variables, whereas the maximum aperture of the control valves is twice the nominal value of the steady state, so in principle the valves are open at 50%. In this manner to build the relative gain matrix, the step change is applied to the manipulated variable and divided by two to have the same range of variation in both closing and opening operation in the control valves. This consideration allows us to relate the amount of change of the manipulated variable with the magnitude of change in control valve which only must vary between 0 and 100%. With this form of scaling it is achieved simultaneously dimensionless standardization and manipulated variables, the term *1/2P* has been included in Eq. (5) in order to accomplish this purpose. Eq. (5) represents the relative gain matrix for the distillation sequences.

$$\begin{bmatrix} K_{11} & K_{12} & K_{13} \\ K_{21} & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{33} \end{bmatrix} = \begin{bmatrix} \frac{x_{C1}^{v_1} - x_{C1}^{sp}}{\frac{1}{2}P} & \frac{x_{C1}^{v_2} - x_{C1}^{sp}}{\frac{1}{2}P} & \frac{x_{C1}^{v_3} - x_{C1}^{sp}}{\frac{1}{2}P} \\ \frac{x_{C2}^{v_1} - x_{C2}^{sp}}{\frac{1}{2}P} & \frac{x_{C2}^{v_2} - x_{C2}^{sp}}{\frac{1}{2}P} & \frac{x_{C2}^{v_3} - x_{C2}^{sp}}{\frac{1}{2}P} \\ \frac{x_{C3}^{v_1} - x_{C3}^{sp}}{\frac{1}{2}P} & \frac{x_{C3}^{v_2} - x_{C3}^{sp}}{\frac{1}{2}P} & \frac{x_{C3}^{v_2} - x_{C3}^{sp}}{\frac{1}{2}P} \end{bmatrix} \tag{5}$$

The elements in the left side of Eq. (5), K_{ij}, are the relative gain matrix. Furthermore, the elements of the first row in the right side correspond to the differences among the mass purity of the component *A* in the nominal state x_A^{sp},and the mass purities after disturbance *p*. $x_A^{V_1}$ is the mass purity of component *A* after disturbance in manipulated variable 1, $x_A^{V_2}$ is the mass purity of component *A* after disturbance in manipulated variable 2, $x_A^{V_3}$ is the mass purity of component *A* after disturbance in manipulated variable 3.

4.4. Multi-objective optimization problem

In the schemes shown in Fig. 1, the target is the simultaneous minimization of the total annual cost (TAC), the environmental impact measured through eco-indicator 99 (EI99) and the condition number (CN). The minimization of these three objectives is subject to the required recoveries and purities in each product stream.

$$\begin{aligned} &\min(TAC, Eco99, \gamma) = f(N_{tn}, N_{fn}, R_{rn}, F_{rn}, F_{ln}, F_{vn}, D_{cn}) \\ &\text{Subject to} \quad \vec{x}_m > \vec{y}_m \end{aligned} \tag{6}$$

where N_{tn} are total number of column stages, N_{fn} is the feed stage in column, R_{rn} is the reflux ratio, F_{rn} is the distillate flux, F_{ln} is the interconnection liquid flow, F_{vn} is the interconnection vapor flow, D_{cn} is the column diameter; y_m and x_m are the vectors of obtained and required purities for the m_{th} components, respectively. Each variable in Eq. (6) has its own role on the objective function calculation. In example, to calculate the total annual cost, it is necessary to sum the capital cost and operating costs. The capital cost depends directly from the column size. With the amount of columns stages it is possible to calculate the high of the column and so on. Moreover if our model is complete with all degrees of freedom such as reflux ratio and distillate flux, we obtain as result the reboiler/condenser duty which allows to calculate those operating cost. On the other hand, in the Eco indicator 99 calculation we consider the impact of steam for heating, steel for equipment building and electricity for pumping. So, with the amount of stages, high of the column, reboiler/condenser duty it is possible to calculate the environmental impact. As concern to the controllability index, note that it is necessary to apply several disturbances in those optimization variables, so as product of those disturbances it is possible to obtain the mass purity of the interest component to eventually calculate the condition number as controllability index. This multi-objective minimization problem has 25 continuous and discrete variables. Note that the product streams flows are manipulated and the recoveries of the key components in each product stream must be included as a restriction/constraints for the optimization problem. Table 3 shows all the decision variables that were used in the process optimization. The physical considerations about the column and equipment size were taken as average industrial measurements concerning distillation column designs [40]. In this work we consider three variables to be used for the control test (the mass purities of acetone, ethanol and butanol) and three manipulated variables (the distillate flow, the side stream flow and the reboiler duty). Note that the size of relative gain matrix is 3 by 3.

5. Global optimization methodology

Stochastic optimization algorithms have proven capable of solving complex optimization problems formulated as mixed integer nonlinear programming (MINLP) models and potentially nonconvex. Note that this type of algorithm has been also used to design and optimize complex schemes [41,42]. Stochastic algorithms can solve robustly the optimization problem with a reasonable computational effort. Moreover, they require only calculation of the objective function and can be used without problem reformulation.

Among stochastic optimization algorithms, Differential Evolution with Tabu List (DETL) has been used in the optimization and design of complex schemes, by Abbas et al. [43]. DETL has its basis in natural selection theory, similar as genetic algorithms. Initially, differential evolution (DE) method was proposed by Storn et al. [44] to solve single objective optimization problems over continuous domains. Afterward, Madavan et al. [45] adapted DE for solving multi-objective optimization problems. Basically, DE algorithm consists of four steps: initialization, mutation, crossover, evaluation, and selection [46]. As a brief description, in the initialization step the algorithm search in a D-dimensional space $\Re^D$, so the initialization of a population starts by randomly generating real-valued parameter vectors. Each vector of a generation *G*, known as genome/chromosome is a candidate solution for the optimization problem, represented as:

$$\vec{X}_{i,G} = [X_{1,i,G}, X_{2,i,G}, X_{3,i,G}, \ldots, X_{D,i,G}] \tag{7}$$

For each parameter involved in the optimization problem there may be a range to limit those vectors proposed. The initial population (at G = 0) should cover this range by prescribing minimum and maximum boundaries $\vec{X}_{i,min} = [X_{1,i,min}, X_{2,i,min}, X_{3,i,min} \ldots, X_{D,i,min}]$ and in such way that the initialized j^{th} component of the i^{th} vector is described as:

$$x_{j,i,0} = x_{j,min} + rand_{i,j}[0,1] \cdot (x_{j,max} - x_{j,min}) \tag{8}$$

Table 3
Decision variables used in the global optimization process.

	Type of variable
Number of stages	Discrete
Amount of mass separating agent	Continuous
Feed stages	Discrete
Side stream stage	Discrete
Side stream flow	Continuous
Reflux ratio	Continuous
Liquid and vapor interconnection flow	Continuous
Stage of liquid and vapor Interconnection flow	Discrete
Distillate rate	Continuous
Diameter	Continuous

In Eq. (8), the function $rand_{i,j}$ is uniformly distributed between 0 and 1, and is instantiated independently for each component of the i-th vector [47].

Regarding to the mutation step, the meaning is indeed similar to biological meaning, mutation is seen in this case as a change or perturbation with a random element. The vector produced by mutation is called *trial* vector. Initially, is necessary to start from a *parent* vector (named *target* vector) of the current generation, this parent vector is muted by the differential mutation operation to generate a *donor* vector, finally an offspring formed by recombining the donor with the target vector we obtain the trial vector. In other words, to create the donor vector, three distinct parameters, $\vec{X}_{r_1^i}, \vec{X}_{r_2^i}$ and $\vec{X}_{r_3^i}$ are sampled randomly from the current population and the sub-index r_1^i, r_2^i and r_3^i are mutually exclusive integers randomly chosen from the range [1, population size]. We can write the process as follows:

$$\vec{V}_{i,G} = \vec{X}_{r^I_{1,G}} + F \cdot (\vec{X}_{r^i_{2,G}} - \vec{X}_{r^i_{3,G}}) \tag{9}$$

In the crossover step, the target vector exchanges its components with the target vector under this operation to form the trial vector $\vec{U}_{i,G} = [u_{1,iG}, u_{2,iG}, u_{3,iG}, \ldots, u_{D,iG}]$. The DE algorithms can use two kind of crossover methods, exponential (also named two-point modulo) and binomial (also named uniform) [47]. In exponential crossover, it is necessary to choose randomly an integer n and L among the range $[1, D]$. Those integers acts as starting point in the target vector, from where the crossover or exchange of components with the donor vector starts. So, the trial vector is obtained as [47]:

$$\begin{aligned} &u_{j,i,G} = v_{j,i,G} \quad for\ j = \langle n \rangle_D \quad \langle n+1 \rangle_{D,\ldots,} \langle n+L-1 \rangle_D \\ &x_{j,i,G}\ for\ all\ other\ j \in [1, D] \end{aligned} \tag{10}$$

Where the angular brackets $\langle - \rangle_D$ denote a module function with modulus D. On the other hand, binomial crossover is carried out on each of the D variables whenever a randomly generated number between 0 and 1 is less or equal than crossover value Cr. The operation may be explained as follow:

$$u_{j,iG} = \begin{cases} u_{j,iG} & if\ (rand_{i,j}[0,1] \leqslant Cr\ o\ j = j_{rand}) \\ x_{j,i,G} & if\ (rand_{i,j}[0,1] > Cr\ y\ j \neq j_{rand}) \end{cases} \tag{11}$$

Concerning the selection step, in order to keep the population size as a constant number over subsequent generation, the selection step determine if the target or the trial vector survives from the generation G to the next generation $G + 1$. The selection operation is described as:

$$\begin{aligned} &\vec{X}_{i,G+1} = \vec{U}_{i,G} \quad if\ f(\vec{U}_{i,G}) \leqslant f(\vec{X}_{i,G}) \\ &\vec{X}_{i,G+1} = \vec{X}_{i,G} \quad if\ f(\vec{U}_{i,G}) > f(\vec{X}_{i,G}) \end{aligned} \tag{12}$$

Where $f(\vec{X})$ is the objective function to be minimized/maximized. Hence, if new trial vector has equal or lower value of the objective function, it replaces the corresponding target vector in the next generation, in another way the target is retained in the population.

On the other hand, Taboo List concept (TL) proposed by Glover et al. [46] and Taboo Search (TS) is included to avoid the revisit of search space by keeping a record of visited points. TL is randomly initialized at initial population and continuously updated with the newly generated trial individuals. This taboo check is carried out in the generation step to the trial vector, and the new trial individual is generated repeatedly until it is not near to any individual in the TL. In this manner the objective functions are evaluated for this new trial individual. The total trial individuals NP are generated by the repetition of above steps. The newly generated NP trial vectors are combined with the parent population to form a combined population with total 2NP individuals. This combined population undergoes non-dominated sorting and ranking accordingly. Individuals with the same non-dominated rank are further ranked on the basis of crowding distance. The first (best) NP individuals are used as the population in the subsequent generation [48].

To perform the global optimization a hybrid platform linking Aspen Plus, Microsoft Exceland Matlab was used. Inside Microsoft Excel, the DETL algorithm is written by means of Visual Basic (VBA) and the entire model of the separation process is rigorously modeled in Aspen Plus. As a brief description of the optimization process, initially the vector of decision variables is sent from Microsoft Excel to Aspen Plus by means of DDE (Dynamic Data Exchange) through COM technology. Those values are assigned to process variables in Aspen Plus modeler. After converging the simulations, Aspen Plus returns to Microsoft Excel a resulting vector containing output data (reboiler heat duty, total stages, etc.). Then disturbances are applied on the manipulated variables and new simulations are executed, after these simulations are completed the differences among the components mass purity in the nominal state and the components mass purity after the disturbances are estimated, these data along with the necessary data to calculate the condition number are sent from Microsoft Excel to Matlab. Finally, Microsoft Excel analyzes the objective function values and proposes new values of decision variables according to the DETL method. In this work, the following parameters for the optimization method have been used: 200 individuals, max. 500 number of generations, a taboo list of 50% of total individuals, a taboo radius of 1×10^{-6}, 0.8 and 0.6 for crossover probability and the mutation factor, respectively. These parameters were obtained from the literature and tuning process via preliminary calculations [49].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 the DETL method.

6. Results and discussion

This section presents the main results of the simultaneous evaluation of the multi-objective function. The optimization fulfills all constrains related to purity and recovery. Before the optimization was performed, all base case designs were modeled and simulated in Aspen Plus using the rigorous RADFRAC unit. Hence all process schemes were robustly designed taking into account the complete set of MESH equations (mass balances, equilibrium relationships, summation constraints, and energy balance).

Figs. 2–4 show the convergence behavior of the objective functions after the optimization. All Pareto fronts were obtained after 100,000 evaluations, as afterward the vector of decision variables did not produce any meaningful improvement. It was assumed that the DETL algorithm achieved the convergence at the tested numerical terms and thus the results reported here correspond to the best solution obtained.

Although in this work three objective functions were evaluated at the same time, for a better understanding of the Pareto fronts we presented first a Pareto front with only two objective functions. Fig. 2 shows the Pareto front evaluating the total annual cost and the condition number. Based on this figure, it is clear that scheme 2 showed the lowest economic impact in comparison with the other three schemes. But in Fig. 2 a clear tendency is observed when both objective functions are evaluated, when the TAC is minimized the control properties measured by the condition number gets worse. In other words, the lowest values of condition number

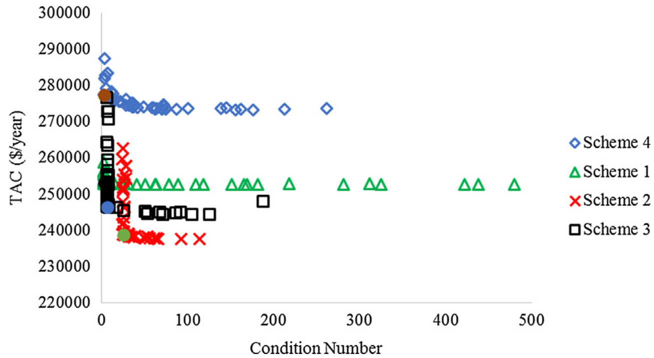

Fig. 2. Pareto front between TAC and condition number for all biobutanol purification schemes.

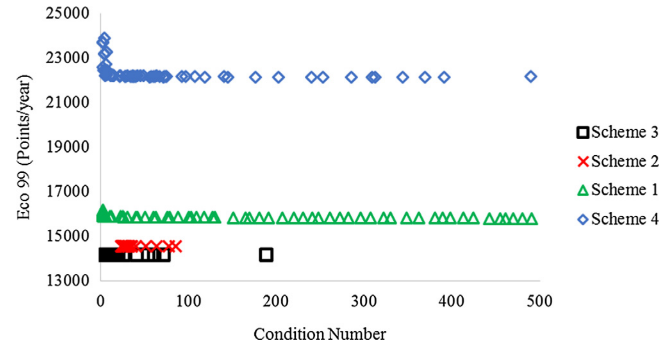

Fig. 4. Pareto front between Eco-indicator 99 and Condition Number for all biobutanol purification schemes.

(i.e. meaning a good dynamic behavior) are obtained at the highest TAC values.

Among all schemes presented in Figs. 2–4, a design was selected for each scheme, for which both objective functions reach a minimum (see highlighted point in Fig. 2). All the variables and parameters for those schemes are presented in Tables 4–7. The selection of those points was carried out considering that actually a feasible zone exists where all objective functions are at minimum, according to the study of Martinez-Iranzo et al. [50]. Taking into account the analysis for Fig. 2, and considering the variables and parameters shown in Tables 4–7, it is evident that the cheapest alternative is scheme 2. This was obtained considering the lowest number of theoretical of equilibrium stages, but the reflux ratio is also the highest of the four schemes. Although the reboiler duty of this scheme is about the same as the rest, note that only one reboiler is used which minimizes the auxiliary equipment cost. Conversely, scheme 4 is the most expensive one, as this process alternative requires the largest amount of heat duty and a larger column diameter, thus having a negative direct impact on the TAC.

Regarding to the controllability, high TAC values are related with low condition number values (meaning that built-in controllability has its cost). DWC are known to have adequate controllability [51]. Among all alternatives, scheme 4 showed the lowest condition number, which means it has the best controllability properties. Observing the parameters from Table 7, scheme 4 has larger column diameters and largest heat duty (e.g. high boil-up ratio and reflux ratio) and this allows the design to reject larger disturbances. In terms of the main difference in CN between the best and worst schemes, the position of the DWC in the process seems to affect the controllability. Scheme 4 (lowest CN) is the only scheme with the DWC positioned as the first separation unit, unlike the other three schemes where the DWC is used as the second separation unit. This issue has been previously discussed by Lucero-Robles et al. [52].

Regarding Fig. 3, where TAC is presented jointly with the Eco-indicator 99, the tendency is that for cheaper schemes EI99 increases as well. The most balanced solution considering only these two objectives would be scheme 3, since its environmental impact is the lowest and the TAC value is second best (after scheme 2). With the largest TAC, scheme 4 showed also the largest environmental impact, since this scheme has largest energy requirements and large equipment that increases the use of steel. This behavior shown in Fig. 3 represents the conflicting targets along the optimization. The upper zone in the Pareto front is obtained by designs which preferably include the largest number of stages, the largest diameter of column but the lowest heat duty (because of the well-known relation among those variables) – these combinations produced the highest TAC value but the smallest eco-indicator 99. The lower area of the Pareto front consists of designs that include a low number of stages, the smallest column diameter, but the largest heat duty – which produced the lowest TAC but the highest eco-indicator 99. At the middle of both zones, it can be assumed that the minimum values of both objective functions coexists, so it includes designs with average variables between both zones, which is reflected in the TAC and eco-indicator 99 values.

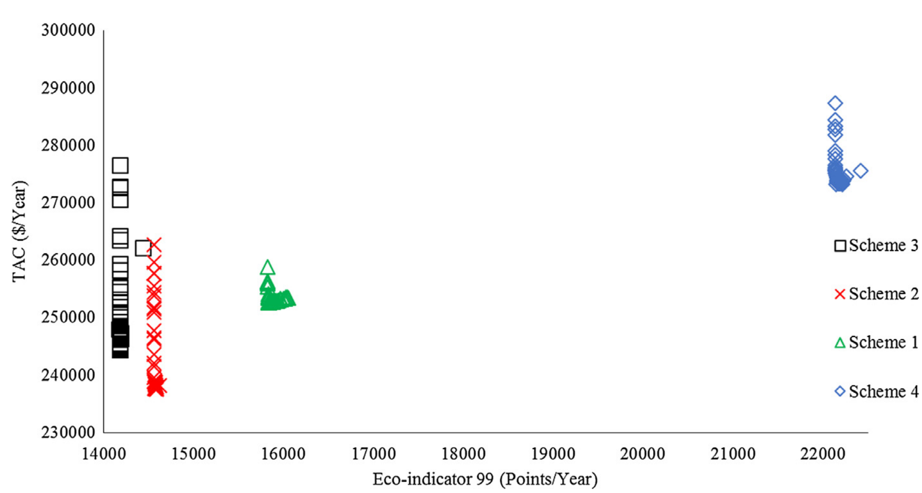

Fig. 3. Pareto front between TAC and Eco-indicator 99 for all biobutanol purification schemes.

Table 4
Design parameters and performance indexes for Scheme 1.

Quantity	Extractor	Column 1	Dividing Wall column	
			Prefractionator	Main Column
Number of theoretical stages	5	27	34	62
Reflux ratio	–	0.3492	–	28.525
Feed stage	1	15	19	–
Interlinking stages		1/1		29/55
Solvent feed stage	5	–	–	–
Side stream stage	–	–	–	49
Column diameter (m)	0.335	0.287	0.296	0.2907
Operative pressure (kPa)	101.353	101.353	101.353	101.353
Distillate flowrate (kg·h^{-1})	–	34.425	–	7.703
Side stream flowrate (kg·h^{-1})	–	–	–	0.328
Liquid split ratio r_L (kg·kg^{-1})	–	–	0.1772	–
Vapor split ratio r_V (kg·kg^{-1})	–	–	0.0882	–
Solvent flowrate (kg·h^{-1})	708.549	–	–	–
Solvent makeup (kg·h^{-1})	0.708	–	–	–
Condenser duty (kW)	–	0	–	32.44
Reboiler duty (kW)	–	64.6809	–	26.81
Total Annual Cost ($/y)	253089			
Eco-indicator 99 (points/y)	15972			
Condition Number	2.65			

Table 5
Design parameters and performance indexes for Scheme 2.

Quantity	Extractor	Column 1	Dividing Wall column	
			Prefractionator	Main Column
Number of theoretical stages	5	35	14	46
Reflux ratio	–	16.706402	–	34.675
Feed stage	1	18	10	–
Interlinking stages		35/35		8/26
Solvent feed stage	5	–	–	–
Side stream stage	–	–	–	17
Column diameter (m)	0.335	0.295	0.365	1.023
Operative pressure (kPa)	101.353	101.353	101.353	101.353
Distillate flowrate (kg·h^{-1})	–	7.704	–	0.312
Side stream flowrate (kg·h^{-1})	–	–	–	13.694
Liquid split ratio r_L (kg·kg^{-1})	–	–	0.6673	–
Vapor split ratio r_V (kg·kg^{-1})	–	–	0.4121	–
Solvent flowrate (kg·h^{-1})	708.549	–	–	–
Solvent makeup (kg·h^{-1})	0.709	–	–	–
Condenser duty (kW)	–	19.525	–	15.254
Reboiler duty (kW)	–	0	–	84.313
Total Annual Cost ($/y)	238783			
Eco-indicator 99 (points/y)	14583			
Condition Number	24.73			

Table 6
Design parameters and performance indexes for Scheme 3.

Quantity	Extractor	Column 1	Dividing Wall column	
			Prefractionator	Main Column
Number of theoretical stages	5	26	33	61
Reflux ratio	–	1	–	12.939
Feed stage	1	14	20	–
Interlinking stages		35/35		24/53
Solvent feed stage	5	–	–	–
Side stream stage	–	–	–	49
Column diameter (m)	0.335	0.301	0.312	0.297
Operative pressure (kPa)	101.353	101.353	101.353	101.353
Distillate flowrate (kg·h^{-1})	–	21.686	–	7.7
Side stream flowrate (kg·h^{-1})	–	–	–	0.3262
Liquid split ratio r_L (kg·kg^{-1})	–	–	0.3018	–
Vapor split ratio r_V (kg·kg^{-1})			0.8748	
Solvent flowrate (kg·h^{-1})	708.549	–	–	–
Solvent makeup (kg·h^{-1})	0.708	–	–	–
Condenser duty (kW)	–	7.646	–	15.309
Reboiler duty (kW)	–	66.281	–	15.752
Total Annual Cost ($/y)	246434			
Eco-indicator 99 (points/y)	14189			
Condition Number	6.63			

Table 7
Design parameters and performance indexes for Scheme 4.

Quantity	Extractor	Dividing Wall column		Column 2
		Prefractionator	Main Column	
Number of theoretical stages	5	19	58	35
Reflux ratio	–	–	7.695	16.706
Feed stage	1	11	–	6
Interlinking stages		30/50	58/58	
Solvent feed stage	5	–	–	–
Side stream stage	–	–	47	–
Column diameter (m)	0.335	1.819	1.484	0.295
Operative pressure (kPa)	101.353	101.353	101.353	101.353
Distillate flowrate ($kg \cdot h^{-1}$)	–	–	0.312	7.704
Side stream flowrate ($kg \cdot h^{-1}$)	–	–	0.32966374	–
Liquid split ratio r_L ($kg \cdot kg^{-1}$)	–	0.4711	–	–
Vapor split ratio r_V ($kg \cdot kg^{-1}$)	–	0.2888	–	–
Solvent flowrate ($kg \cdot h^{-1}$)	708.549	–		–
Solvent makeup ($kg \cdot h^{-1}$)	0.709	–	–	–
Condenser duty (kW)	–	–	13.218571	62.406
Reboiler duty (kW)	–	–	0	135.685
Total Annual Cost ($/y)	277383			
Eco-indicator 99 (points/y)	23669			
Condition Number	2.41			

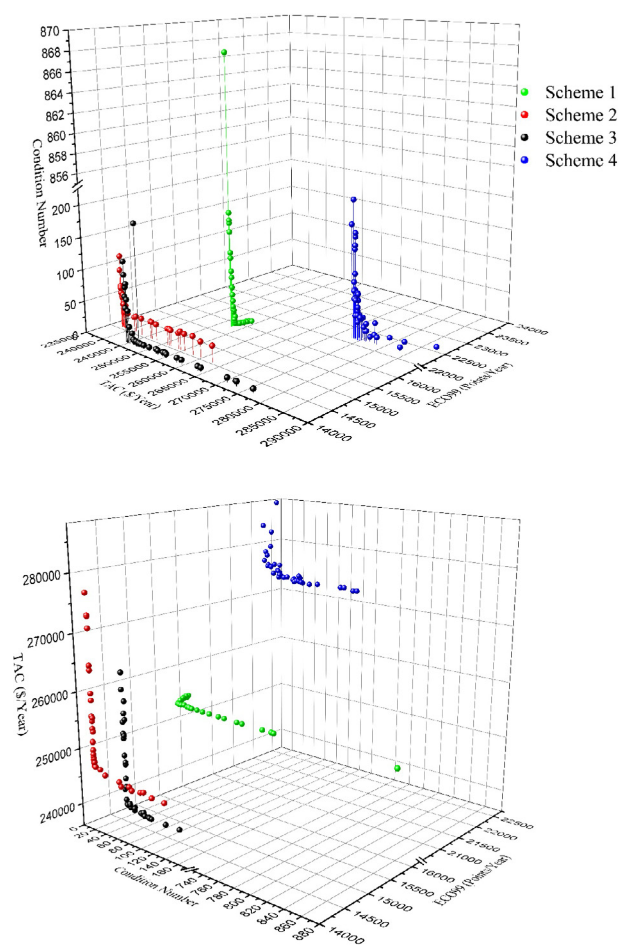

Fig. 5. Pareto front between TAC, Eco-indicator 99 and Condition Number for all biobutanol purification schemes.

Fig. 4 shows the Pareto front for the condition number and eco-indicator 99. As reminder, the eco-indicator 99 calculations consider the impact of steam, steel and electricity – among these impact factors the steam production is the most weighted (Table 2). Consequently, in Fig. 4 the highest value of eco-indicator 99 corresponds to scheme 4 (highest energy use, but lowest condition number). This behavior is consistent with previous results, where a direct relation was assumed between the energy use and the condition number values. However, scheme 2 (lowest TAC) apparently could be the scheme with the lowest environmental impact since one can assume that the cheapest alternative has the lowest energy usage. Nonetheless, Figs. 3 and 4 confirm the contrary. The slight difference in eco-indicator 99 between scheme 2 and scheme 3 is due to the size of diameter on each column (see Tables 4–7) since the steel to build all equipment is also included in EI99.

The 3-D Fig. 5 shows the evaluation of the optimization carried out by evaluating all three objective functions at the same time. Clearly, there are some conflicts to be solved during optimization. To minimize the TAC, the optimization method is always searching for the lowest energy use and at the same time the lowest number of stages and smaller diameters (which actually are in conflict with each other). However, the tendency of the Pareto front shows that with cheaper and smaller equipment the control properties get worse. Hence it is necessary to find a trade-off between those two objective functions. The condition number is related to the size of the column and energy usage to purify the mixture, but if those variable values increase then the environmental impact increases too, so a balance of those objectives is needed. In other words, the columns size, energy use and design variables for those three objective functions are in conflict. The crowded zone in Fig. 5 represents the most feasible zone where the three objective functions find a trade-off solution.

Concerning the total annual cost, scheme 2 allows savings of about 4%, 6% and 18% as compared to scheme 3, 1 and 4, respectively. In terms of control properties, scheme 4 showed the best controllability index, improving with 8%, 65% and 90% as compared to scheme 1, 3 and 2, respectively. Regarding the environmental impact, scheme 3 showed the lowest impact with 3%, 11% and 47% reduction as compared to the scheme 2, 1 and 4, respectively. The analyzed schemes 1–4 show a specific energy use of 24.54, 22.19, 21.59, 35.73 MJ per kg butanol, respectively (see Fig. 6 for a complete mass/energy balance scheme). In this respect, scheme 3 has the best performance. As preliminary conclusion the intensified systems are always aimed to improve energy efficiency, however for the current intensified systems studied, the higher savings in TAC, the poorer the dynamic response. So, in the continuous

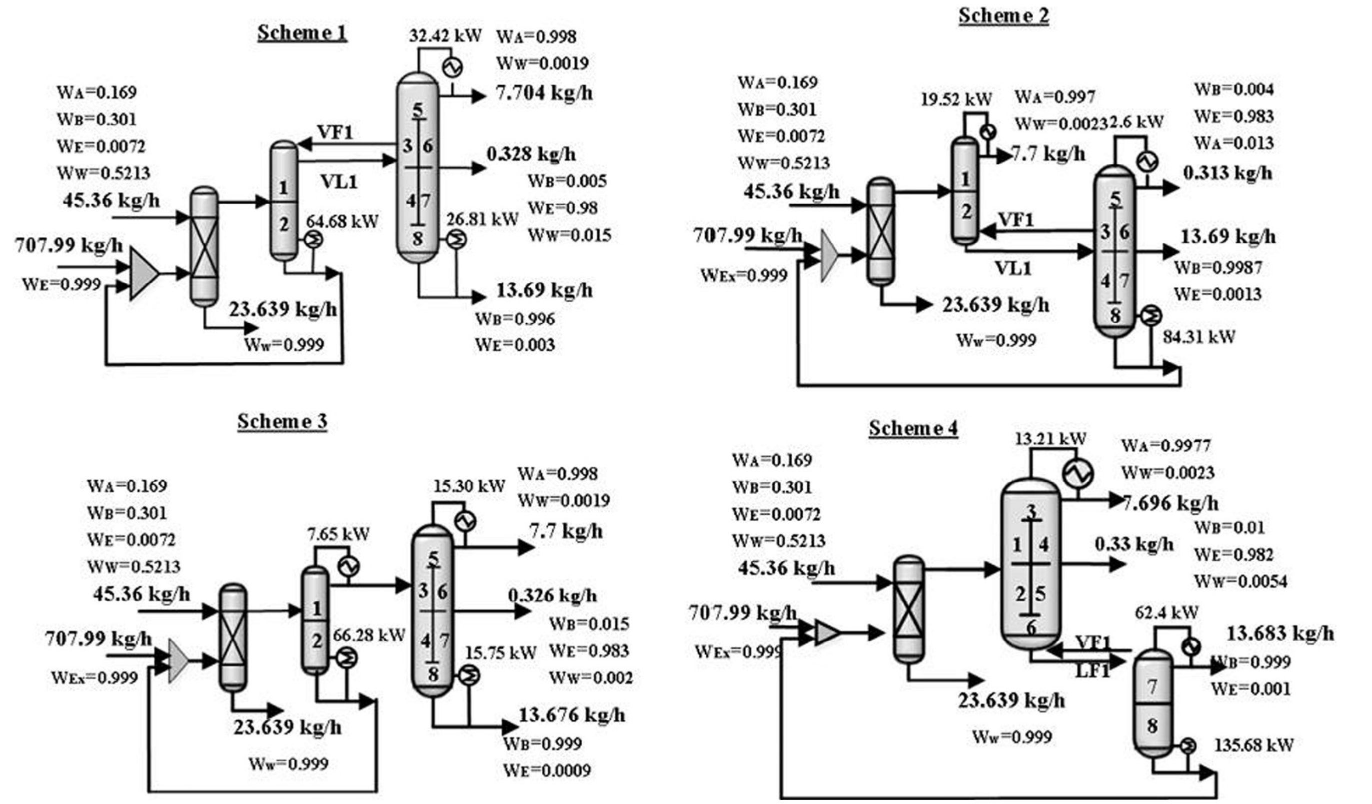

Fig. 6. Mass/energy balances for all analyzed schemes.

search to find better values for condition number, some other energetic or economic indexes are sacrificed and vice versa. This behavior agrees up to certain extent with the literature [53–55]: highly intensified systems (aiming at minimizing energy consumption under specific designs) imply a high degree of nonlinearity and interaction between variables, and loss of control degrees of freedom that restrict the operating conditions flexibility of the system, so the feasibility to find a good dynamic behavior zone it depends totally of a correct addressing as concern to energy consumption .

7. Conclusions

The hybrid schemes proposed in this work were evaluated using multi-objective optimization with three functions: total annual cost (TAC), the eco-indicator 99 and the condition number representing the economic, environmental and controllability indexes, respectively. Scheme 2 proved to have the most balanced design among the four schemes evaluated, as it showed the lowest TAC values, as well as relatively low condition number and eco-indicator 99 values. It was also observed that the column size and energy use affect directly the controllability, economic and environmental impact indexes.

The optimal solution found is a trade-off between those characteristics, column size and energy use which should be not so large (to minimize TAC and eco-indicator 99 respectively) but sufficiently high for good controllability properties. In general, this design methodology allows the designer to choose the right option considering more complete scenarios taking into account not only the economic and environmental impact, but also having a preliminary measure of the controllability properties. This kind of research efforts, combined with results of other research areas, can lead to a profitable ABE fermentation process able to compete with traditional ways to produce biobutanol fuel.

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