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A hybrid model of multi-objective differential evolution algorithm and various decision-making methods to optimize the batch ABE fermentation process

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Abstract. In recent years, biofuels have attracted considerable attention as a renewable and clean source of energy and have been playing the role of suitable alternatives to fossil fuels. One of the most attractive types of biofuels is Acetone-Butanol-Ethanol (ABE), which is produced in a batch fermentation process by the anaerobic bacterium *Clostridium acetobutylicum* and sugar-based substrate as feedstock. In this paper, the optimization of this process was carried out according to a bi-objective function. A hybrid model of Multi-Objective Differential Evolution (MODE) algorithm and distinguished decision-making methods, namely linear programming technique for multidimensional analysis of preference (LINMAP), Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS), and Shannon's entropy, were applied to find the final optimal operating point. The initial concentration of substrate and the final operating time of the process were selected as decision variables to maximize the two main objectives in terms of solvent yield and productivity. A Pareto optimal set presents a wide range of optimal operating points, and a proper operating condition can be selected based on the necessities of the applicant. The best optimal point obtained by TOPSIS, according to the lowest value of deviation index, was also compared with the results of the economy-based optimization.

1. Introduction

Due to the rapid depletion of fossil fuel resources and the serious concerns over environmental pollution resulting from petroleum fuel emissions, the demand for biofuels is rising. Biobutanol is a valuable biofuel that can be used as a direct substitution of gasoline or as a fuel additive. Besides, butanol is used as a solvent in chemical industries and as an intermediate in chemical synthesis and pharmaceutical manufacturing. In recent years, due to the increasing petroleum prices and energy requirement, cheaper separation technology, and growing demand for renewable energy resources, the ABE fermentation process as a common way to produce butanol has been taken into account [1].

ABE can be synthesized biologically by the anaerobic bacterium *Clostridium acetobutylicum* and produces three solvents (acetone, butanol, and ethanol), two intermediate metabolites (butyric acid and acetic acid), and two gases (carbon dioxide and hydrogen) [2]. In the ABE bioreactor, the substrate is the glucose syrup. The metabolic pathway of ABE production is divided into two separate phases: acidogenesis and solventogenesis. During the acidogenesis phase, the

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bacterial culture mainly produces butyric and acetic acids and, during the solventogenic phase, acetic and butyric acids are converted to acetone and butanol, respectively [3].

To improve the performance of the ABE process, it is required to implement the process under optimal conditions by considering economic feasibility and safety. Several research studies have been conducted on the optimization of the ABE fermentation process for high butanol production. These studies can be divided into two categories: mathematical model-based optimization and experimental design-based optimization.

Extensive studies have been performed on the optimization of the ABE process in the fed batch and continuous reactors based on the mathematical model, which are presented as follows. Dynamic optimization of the semi-batch ABE fermentation with *in situ* pervaporation membrane separation was accomplished by Lin and Lee [4] to determine the optimal feeding profile through time. Sandu et al. [5] selected the substrate concentration, the inoculum volume, and the feed flow rate as decision variables to maximize the production of solvents in the ABE fed-batch biosynthesis. Grisales-Diaz and Olivar-Tost [6] optimized economically a process involving simultaneous saccharification, ABE fermentation from lignocellulose, and detoxification by liquid-liquid extraction using a simplex search method. Elmeligya et al. [7] proposed an artificial neural network as a metamodel for optimizing the biobutanol production process via the integrated ABE fermentation-membrane pervaporation process. Kim et al. [8,9] suggested a model-based optimization strategy for the ABE fermentation process coupled with an ex-situ recovery system with periodically switched adsorption column for continuous biobutanol production. The Sequential Quadratic Programming (SQP) algorithm was used to search the optimal operating conditions, leading to the most profitable cyclic steady state. Mariano et al. [10,11] performed a dynamic optimization for the continuous ABE fermentation process containing a fermentor, a cell retention system, and a vacuum flash vessel to maximize the butanol productivity using Particle Swarm Optimization (PSO) and SQP algorithms. Sharma and Rangaiah [12] optimized a three-stage fermentation process, which is integrated with cell recycling and inter-stage extraction for ethanol productivity and xylose conversion using MODE algorithm. Sharif Rohani [13] implemented the multi-objective optimization for the ABE continuous process coupled with an *in situ* separation unit, namely vacuum fermentation, gas stripping, and pervaporation, to determine the optimal operating conditions. The butanol specific productivity, average butanol concentration, and sugar conversion were selected as objective functions. The Pareto-optimal solutions obtained by Genetic Algorithm (GA) were ranked by the Net Flow Method (NFM) to find the best point.

Generally, the experimental design-based optimization (second category) was carried out by several researchers using Response Surface Methodology (RSM) [14,15]. Wang and Blascheck [16] performed batch experiments by Central Composite Design (CCD) [15] and RSM optimization to evaluate the effect of initial glucose concentration, agitation rate, and PH on butanol production. YouSheng et al. [17] optimized experimental conditions for the production of butanol in a batch bioreactor based on enzymatic hydrolysis of corn stalk by adopting Plackett-Burman Design (PBD) [18] and CCD to screen the key factors. Singh et al. [19] used PBD and RSM methodology to optimize fermentation medium for enhancing butanol production from glucose by *Clostridium beijerenckii* strain CHTa. Optimization of the ABE batch process parameters containing acid concentration, temperature, incubation time, algal hydrolysate concentration, inoculum size, and initial pH was carried out by Dubey et al. [20] to enhance biobutanol production from *Sargassum wightii* hydrolysate. Kumar et al. [21] suggested the utilization of the agro residue corncob for the production of the ABE using *Clostridium acetobutylicum* and optimized this batch bioreactor through RSM. Zheng et al. [22] enhanced the ABE production from eucalyptus hydrolysate with optimized nutrient supplementation containing $FeSO_4.7H_2O$, tryptone, and yeast extract through statistical experimental designs. Al-Shorgani et al. [23-25] used PBD to optimize the batch ABE culture conditions in order to screen the most significant factors affecting the biobutanol production by various anaerobic bacteria. Recently, Khunchantuek and Fiala [26] and Sirisantimethakom et al. [27] investigated the optimization of the various key factors affecting butanol production from sugarcane juice and sweet sorghum stem juice, respectively, by *Clostridium beijerinckii* TISTR 1461 using RSM.

Continuous and fed-batch cultures are alternatives for the ABE process, yet with their own intrinsic disadvantages. The ABE fermentation was implemented widely in the batch reactor during its commercial production years. The batch fermentation is easier to operate and less likely to be contaminated [28]. According to the content mentioned in the previous paragraph, all studies on the optimization of the ABE batch process are based on the experimental design. To the best knowledge of the authors, this is the first time the optimization of the ABE batch fermentation process has been conducted based on a mathematical model. In this regard, it is essential to assess the response of optimization techniques for the ABE fermentation process, which can be a very effective tool in the search for economic feasibility of the ABE fermentation plants by operating under optimal conditions.

In 1997, the Differential Evolution (DE) algo-

Table 1. The kinetic rates for the batch ABE fermentation process proposed by Votruba et al. [2].

Equation	Definition
$r_X = \lambda(y(t)-1)C_X(t) - k_2 C_X(t) C_B(t)$	Rate of biomass growth
$r_S = -k_3 C_S(t) C_X(t) - k_4 \frac{C_S(t)}{k_s + C_S(t)} C_X(t)$	Rate of substrate utilization
$r_{BA} = k_5 C_S(t) \frac{k_I}{k_I + C_B(t)} C_X(t) - k_6 \frac{C_{BA}(t)}{k_{BA} + C_{BA}(t)} C_X(t)$	Rate of butyric acid production
$r_B = k_7 C_S(t) C_X(t) - 0.841 r_{BA}$	Rate of butanol production
$r_{AA} = k_8 \frac{C_S(t)}{k_S + C_S(t)} \frac{k_I}{k_I + C_B(t)} C_X(t) - k_9 \frac{C_{AA}(t)}{k_{AA} + C_{AA}(t)} \frac{C_S(t)}{k_S + C_S(t)} C_X(t)$	Rate of acetic acid production
$r_A = k_{10} \frac{C_S(t)}{k_S + C_S(t)} C_X(t) - 0.484 r_{AA}$	Rate of acetone production
$r_E = k_{11} \frac{C_S(t)}{k_S + C_S(t)} C_X(t)$	Rate of ethanol production
$r_{CO_2} = k_{12} \frac{C_S(t)}{k_S + C_S(t)} C_X(t)$	Rate of carbon dioxide production
$r_{H_2} = k_{13} \frac{C_S(t)}{k_S + C_S(t)} C_X(t) + k_{14} C_S(t) C_X(t)$	Rate of hydrogen production

rithm for solving optimization problems was proposed by Storn and Price [29] for the first time. The DE method is a stochastic optimization algorithm for minimizing an objective function subject to a number of linear or nonlinear constraints. DE has been successfully used by several researchers such as Babu et al. [30-32] and Khademi et al. [33-36] in various fields. After that, MODE algorithm, as an extended DE method, proposed by Babu et al. [37] has been successfully used to handle multi-objective optimization problems.

In this paper, a dynamic mathematical model is considered for the ABE batch fermentation process. The model is implemented with the aim of identifying important parameters containing an initial concentration of substrate and operating time affecting the biosynthesis of products in the fermentation process. A study on the optimization of ABE fermentation process is carried out according to two categories: (1) A multi-objective optimization using the MODE algorithm as an exceptionally simple evolution strategy. In this way, an optimum value is selected from the Pareto-optimal front using a set of decision-making tools, namely TOPSIS [38], LINMAP [39], and Shannon's entropy [40] methods, based on deviation index, and (2) An economy-based optimization using the DE algorithm.

Table 2. Constants for the kinetic model proposed by Votruba et al. [2].

Parameter	Value	Unit
k_1	0.0090	L/g substrate.h.
k_2	0.0008	L/g butanol.h
k_3	0.0255	L/g biomass.h
k_4	0.6764	g substrate/g biomass.h
k_5	0.0136	g butyric acid / L/g substrate g biomass h
k_6	0.1170	g butyric acid/g biomass. H
k_7	0.0113	g butanol / L/g substrate / g biomass H
k_8	0.7150	g acetic acid/g biomass.h
k_9	0.1350	g acetic acid/g biomass.h
k_{10}	0.1558	g aceton/g biomass.h
k_{11}	0.0258	g ethanol/g biomass.h
k_{12}	0.6139	g CO_2/g biomass.h
k_{13}	0.0185	g H_2/g biomass.h
k_{14}	0.00013	g H_2.L/g substrate.g biomass.h
k_I	0.833	g butanol/L
k_S	2.0	g substrate/L
k_{AA}	0.5	g acetic acid/L
k_{BA}	0.5	g butyric acid/L
λ	0.56	–

2. Mathematical model

The mathematical model represents the biochemical kinetics and culture-related physiological aspects of the batch ABE fermentation process. The kinetic model used in this study was developed by Votruba et al. [2] based on the following assumptions: (i) There are no culture restrictions by phosphate, nitrogen, trace elements, and growth factors; (ii) Sugar (glucose) is the only limiting substrate in the batch fermentation process. The mathematical modeling accomplished by other researchers such as Yerushalmi et al. [41,42], Mulchandani and Volesky [43], Srivastava and Volesky [44], and Sandu et al. [5] is on the basis of the kinetic model proposed by Votruba et al. [2].

The kinetic rates for the batch culture are summarized in Table 1. These equations represent kinetic rates for the biomass, substrate, intermediate compounds, and key products (acetone, butanol, and ethanol). The constants that appear in kinetics expressions are tabulated in Table 2.

A hyperbolic relation for product inhibition and a linear relation of the culture physiological state (y) with respect to substrate concentration are added to this model. Variation of y versus time was reported by

Votruba et al. [2] as follows:

$$\frac{dy(t)}{dt} = \left[k_1 C_S(t) \frac{k_{\mathrm{I}}}{k_{\mathrm{I}} + C_B(t)} - \lambda(y(t) - 1)\right] y(t). \quad (1)$$

A differential mass balance equation to describe the dynamic of the process is expressed as follows:

$$\frac{dC_i(t)}{dt} = r_{\mathrm{i}}(t), \quad (2)$$

where i denotes biomass (X), glucose (S), butanol (B), acetone (A), ethanol (E), Butyric Acid (BA), Acetic Acid (AA), carbon dioxide (CO_2), and hydrogen (H_2).

3. Optimization

3.1. Differential evolution algorithm

Differential Evolution (DE) is an effective intelligent optimization algorithm and a population-based stochastic search method. This technique has been presented as an efficient, fast, robust, and simple method for stochastic global optimization. The main algorithm of DE can be found in the literature [37,45], and it consists of a four-step procedure: (1) random choice of an initial population vector, (2) mutation/perturbation (3) crossover/recombination, and (4) selection.

3.2. Various strategies of DE

The DE algorithm can support various strategies depending on the specific problem applied. Related strategies can be different based on the vector to be mutated, the number of difference vectors selected for mutation, and finally the pattern of the recombination used. Ten various strategies with the symbolic form $DE/x/y/z$ were designed by Price and Storn [46]. DE stands for differential evolution, x denotes the vector to be mutated that can be the best member of the previous population or can be selected at random (best or rand, respectively), y represents the number of difference vectors for mutation of x (1 or 2), and z stands for the type of the recombination used (exp: exponential; or bin: binomial). In this study, DE/best/1/bin strategy is used due to its simple form and performance.

3.3. Choosing DE parameters

Some general instructions are available for selecting the crucial parameters such as crossover probability constant (CR), population size (NP), and scaling factor (F) that affect the performance of DE. Mostly, population size must be roughly 5-10 times the number of decision variables [30]. F is situated in the domain of 0.4 to 1.0. At first, a scaling factor equal to 0.5 can be tested; then, F and/or NP increase(s) if the population converges before the usual time. Moreover, CR should be in the range of 0.1 to 1.0 [30]. More aspects of the pseudo-code of DE, its strategies, and the parameters were published by Babu and Munawar [30] and Babu and Angira [31,32]. In the present work, the strategy and parameters used for DE are presented in Table 3.

Table 3. Strategy and parameters applied to DE.

Strategy	DE/best/1/bin
Population size (NP)	50
Scaling factor (F)	0.8
Crossover probability constant (CR)	1
Number of generations	300

3.4. Multi-Objective Differential Evolution (MODE)

Simultaneous optimization of several objectives can be performed by either a single-objective function, in which a weighted average is used for a combination of the individual objectives (known as the weighted-sum method) or multi-objective functions capable of supporting the simultaneous optimization of two or more incompatible objectives [47]. Such objective functions are often in conflict with each other. The trade-off between multiple objectives creates a set of optimal solutions, namely "Pareto-set". The MODE, which is an extension of DE, is used to solve the multi-objective optimization problems.

Figure 1 presents the steps involved in the MODE algorithm. The algorithm can be summarized as follows: An initial population is randomly generated in the feasible region. All dominated points are eliminated from the population. The rest of the non-dominated points are maintained for crossover and are allowed to undergo DE operations. Three parent vectors are randomly chosen. A child vector is created from the three-parent vectors and is put into the population if it dominates the first parent vector; otherwise, a new selection process has been accomplished [45]. The termination criterion of this procedure is an assigned number of generations. A detailed representation of MODE algorithm using DE approach and the general pseudo-code for MODE can be found in the literature [37,48].

3.5. Optimization problem formulation

In this study, two types of the optimization problem are considered: multi-objective optimization and economy-based optimization. In the economy-based optimization, practically, the value of a bio-species can vary significantly, sometimes from one to ten-fold, depending on the economical evaluation methods. Therefore, the results of the economy-based optimization severely depend on the value of species over time. Instead, a multi-objective optimization considerably increases the role of a decision-maker to select the optimal point from the Pareto-set, and its results do not change over the

$$\begin{array}{lll} \text{Maximize}: & f_1(C_S^0, t_f) = 2Y_{\mathrm{A}}(t_f) + Y_{\mathrm{B}}(t_f) + 6Y_{\mathrm{E}}(t_f) & \\ C_s^0, t_f & f_2(C_S^0, t_f) = 2P_{\mathrm{A}}(t_f) + P_{\mathrm{B}}(t_f) + 6P_{\mathrm{E}}(t_f) & \\ \text{Subject to}: & \text{Equation } (i), & i = 1, 2 \\ \text{and} & 0 \leq C_S^0 \leq 150 \text{ gL}^{-1} & \\ & 10 \leq t_f \leq 48 \text{ h} & \end{array} \quad (3)$$

Box I

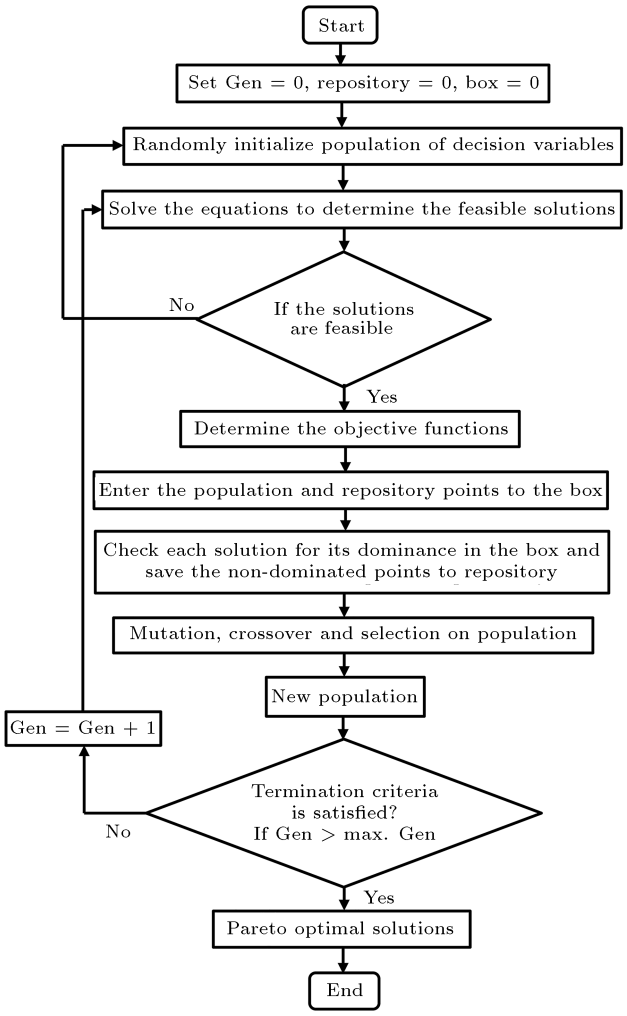

Figure 1. Flowchart of the MODE algorithm.

years. Nevertheless, both optimizations are performed and their results are compared together.

3.5.1. Bi-objective optimization

In this process, 6 variables including yield and productivity of acetone, butanol, and ethanol can be considered as objective functions; however, since it is difficult to discuss and visualize the optimal results of 6 objectives, the number of objectives is reduced to 2 by weighting. The weighted-sum method is applied to each function. A general form of this constrained optimization problem is obtained by Eq. (3) as shown in Box I.

The 3:6:1 solvent concentration ratio of acetone, butanol, and ethanol is commonly observed at the final stage of the batch ABE fermentation process by *C. acetobutylicum* [3,49]. In other words, $C_B/C_E \cong 6$ and $C_B/C_A \cong 2$. Therefore, the objective functions f_1 and f_2 are considered, i.e., the summation of the solvent yield and productivity with weighting factors of 2, 1, and 6 for acetone, butanol, and ethanol to equalize the orders of the magnitude of each term. Eqs. (1) and (2) and the kinetic rates represented in Table 1 are the equality constraints of this problem.

Two decision variables including the initial concentration of substrate, C_s^0, and final operating time of batch fermentation process, t_f, are considered for maximizing these two objective functions. Since C_s^0 is an important parameter and has a direct effect on the solvent yield, this variable is chosen as a decision variable. The range of this parameter is selected based on the information in the literature [2,50]. Functional relationships presented by Votruba et al. [2] for the batch ABE fermentation are reliable for the glucose concentration in the range of 0-50 gL $^{-1}$. Moreover, butanol production was studied by Nanda et al. [50] with glucose as a control substrate at levels varying from 50-150 gL^{-1}. Therefore, an upper bound of 150 gL^{-1} is chosen for the initial concentration of substrate.

In order to allow for cell growth and solvent production, fermentation time was set to 48 h. In the incomplete fermentation of ABE, the process was allowed to proceed for another 48 h. No further changes were observed during this additional time, as reported by Yerushalmi and Volesky [51]. Therefore, the upper bound of the final operating time is set to 48 h. The lower bound for the final operating time has been selected with no prior intention.

3.5.2. Profit function

A simplified profit function is considered as a single-objective function for the economy-based optimization of the batch biological reactor. This constrained optimization problem is generally formulated obtained by Eq. (4) as shown in Box II, where N_A is the

$$\begin{array}{lll} \text{Maximize:} & \text{Profit}(C_S^0, t_f) = 10^{-3}\left(\dfrac{365\times 24}{t_f + t_c}\right)\left\{\begin{array}{l} C_A(t_f)N_A + C_B(t_f)N_B + \\ C_E(t_f)N_E - (C_S^0 - C_S(t_f))N_S \end{array}\right\} & \text{US\$L}^{-1}\text{year}^{-1} \\ C_s^0, t_f & & \\ \text{Subject to :} & \text{Equation } (i), \quad i = 1, 2, & \\ \text{and :} & 0 \le C_S^0 \le 150 \text{ gL}^{-1} & \\ & 10 \le t_f \le 48 \text{ h}, & \end{array} \tag{4}$$

Box II

price of acetone (=US\$0.38 kg^{-1}), N_B is the price of butanol (=US\$0.34 kg^{-1}), N_E is the price of ethanol (=US\$0.28 kg^{-1}), N_S is the price of glucose. Economic calculation is carried out based on the production of ABE from corn. The prices of corn, acetone, ethanol, and butanol are the same as those assumed by Qureshi and Blaschek [52]. Corn of 5.14×10^8 kg (moisture 14%) will result in 3.65×10^8 kg glucose; in addition, the price of corn is considered US\$0.07923 kg^{-1} [52]. Therefore, the price of glucose is US\$0.111 kg^{-1}. Of note, the profit function does not include the cleaning cost in each cycle, bacterial culture and nutrition costs, and separation costs in the separation of by-products (acetic acid and butyric acid) from the ABE and unreacted materials.

4. Decision-making method

The process of decision-making is necessary for selecting the best optimal solution from available points located at Pareto-set. In this research, three decision-making approaches including LINMAP, TOPSIS, and Shannon's entropy are used. Before implementing any decision-making process, it is compulsory to unify the scale and dimension of all the objectives by one of the Euclidean, linear, or fuzzy non-dimensioned methods [53].

4.1. Euclidian approach

In this study, the solvent yield has no unit while the unit of solvent productivity is gL^{-1} h^{-1}. The non-dimensionalized Euclidean approach is applied to unify the dimension of these objective functions as follows [53]:

$$F_{kj} = \frac{f_{kj}}{\sqrt{\sum_{k=1}^{m}(f_{kj})^2}} \qquad j = 1, 2, \tag{5}$$

where F_{kj} is the element of non-dimensionalized objective matrix, f_{kj} is the element of the objectives matrix at various optimal solutions of the Pareto-optimal front, k is the index of various points on Pareto front, m is the total number of points on Pareto front, and j stands for the index of each objective.

4.2. LINMAP method

In the multi-objective optimization, the ideal solution does not lie on the Pareto-set. An ideal solution is a point that optimizes each objective regardless of other objectives. In the LINMAP decision-making approach, the Euclidian distance of each solution on the Pareto-set from the ideal solution, D_k^{ideal}, is computed as follows:

$$D_k^{\text{ideal}} = \sqrt{\left(F_{k1} - F_1^{\text{ideal}}\right)^2 + \left(F_{k2} - F_2^{\text{ideal}}\right)^2}, \tag{6}$$

where F_1^{ideal} and F_2^{ideal} are the ideal solutions for f_1 and f_2. In the LINMAP approach, the point with minimum distance from the ideal solution is chosen as a desired ultimate solution [54]; therefore, $k_{\text{final}} = \arg\min_k(D_k^{\text{ideal}})$.

4.3. TOPSIS method

In the TOPSIS decision-making approach, a non-ideal solution in addition to the ideal solution is considered.

$$D_k = \frac{D_k^{\text{non-ideal}}}{D_k^{\text{ideal}} + D_k^{\text{non-ideal}}}, \tag{7}$$

$$D_k^{\text{non-ideal}} = \sqrt{\left(F_{k1} - F_1^{\text{non-ideal}}\right)^2 + \left(F_{k2} - F_2^{\text{non-ideal}}\right)^2}, \tag{8}$$

where $D_k^{\text{non-ideal}}$ is the Euclidian distance between each point and non-ideal solution, and $F_1^{\text{non-ideal}}$ and $F_2^{\text{non-ideal}}$ are the non-ideal solutions for f_1 and f_2, respectively. The TOPSIS approach computes the final solution on Pareto front with maximum D_k [55]; therefore, $k_{\text{final}} = \arg\max_k(D_k)$.

4.4. Shannon's entropy method

Shannon's entropy method is established based on the weight of each objective function. The linear normalization of the jth objective for the kth point, L_{kj}, is evaluated as follows:

$$L_{kj} = \frac{F_{kj}}{\sum_{k=1}^{m} F_{kj}} \qquad k = 1, 2, \ldots, m \qquad j = 1, 2, \tag{9}$$

$$DD_j = 1 + \frac{\sum_{k=1}^{m} L_{kj} \ln L_{kj}}{\ln(m)}, \tag{10}$$

$$W_j = \frac{DD_j}{\sum_{j=1}^{2} DD_j}, \tag{11}$$

$$S_{kj} = W_j L_{kj}. \tag{12}$$

Shannon's entropy decision-making approach computes the final desired optimal solution on Pareto-set based on the maximum S_k [40]; hence, $k_{\text{final}} = \arg\max_k(S_{kj})$.

4.5. Deviation index

A criterion for selecting a final optimal solution from the optimum points obtained by LINMAP, TOPSIS, and Shannon's entropy decision-making methods is 'Deviation Index' (DI). The deviation index of optimal outcome with respect to the ideal and non-ideal solutions can be given as follows:

$$DI_1^i = \sqrt{\left(F_1^i - F_1^{\text{ideal}}\right)^2 + \left(F_2^i - F_2^{\text{ideal}}\right)^2}, \tag{13}$$

$$DI_2^i = \sqrt{\left(F_1^i - F_1^{\text{non-ideal}}\right)^2 + \left(F_2^i - F_2^{\text{non-ideal}}\right)^2}, \tag{14}$$

$$DI^i = \frac{DI_1^i}{DI_1^i + DI_2^i} \qquad i = 1, 2, 3, \tag{15}$$

where DI^i represents the deviation index of optimal point for the ith decision-making approach ($i = 1, 2$, and 3 denote the LINMAP, TOPSIS, and Shannon's entropy decision-making methods, respectively). The final optimal solution from the Pareto-set and the more appropriate decision-making technique is recognized with the lowest value of the deviation index [56]; therefore, $i_{\text{final}} = \arg\min_i(DI^i)$.

5. Numerical solution

The mathematical model of the batch culture consisting of 10 Ordinary Differential Equations (ODEs) (see Eqs. (1) and (2), as well as Table 1) and the relevant initial conditions generated an initial value problem. The initial conditions are $C_X^0 = 0.03$ gL^{-1}, $C_S^0 = 50$ gL^{-1}, and $y^0 = 1$; the concentration of other components is equal to zero. The ODEs with the initial conditions are simultaneously solved by the Runge-Kutta method of the fourth order in the MATLAB programming environment.

6. Results and discussion

In this section, dynamic behavior and effect of the initial substrate concentration on the performance of the batch bioreactor are investigated. The performance of the bioreactor is analyzed in terms of solvent yield, substrate conversion, and solvent productivity as follows:

$$\text{Solvent yield} = \frac{C_{\text{solvent}}(t)}{C_S^0}, \tag{16}$$

$$\text{Substrate conversion} = \frac{C_S^0 - C_S(t)}{C_S^0}, \tag{17}$$

$$\text{Solvent productivity} = \frac{C_{\text{solvent}}(t)}{\text{Fermentation time}}. \tag{18}$$

6.1. Model validation

In Figure 2, the mathematical model is validated against the experimental data reported by Votruba et al. [2]. This validation is carried out for the solvents, sugar, and biomass concentrations. It is observed in Figure 2 that the batch model agrees well with the experimental data.

6.2. Effect of the initial concentration of substrate

Figure 3(a) and (b) show the effect of the initial concentrations of substrate 25, 50, 100, and 150 gL^{-1} on the butanol and acetone yield, respectively, at various operating times. At a constant initial concentration of substrate, the solvent yield increases until the reaction rate approaches zero. According to Figure 3(a), increasing the initial concentration of substrate from 25 to 150 gL^{-1} leads to an increase in the butanol yield from 0.16 to 0.31 (nearly two folds) in the stationary non-equilibrium state. The increasing rate of butanol yield increases rapidly with an initial concentration of substrate. As seen in Figure 3(b), the acetone yield in the stationary non-equilibrium state increases to reach a certain value and, then, begins to decrease as a result of increasing the initial concentration of glucose from 25 to 150 gL^{-1}. This could be due to butanol inhibition/toxicity and, also, the inhibitory effect of the substrate. Behavior similar to the trend of acetone yield occurs for the ethanol yield at different initial concentrations of substrate. Therefore, C_S^0 has a large

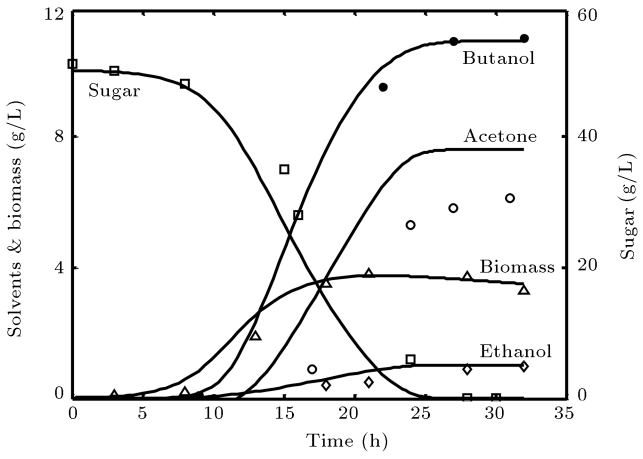

Figure 2. Comparison between simulation results (solid lines) and experimental data (marker) reported by Votruba et al. [2] for $C_X^0 = 0.03$ gL^{-1}, $C_S^0 = 50$ g L^{-1}.

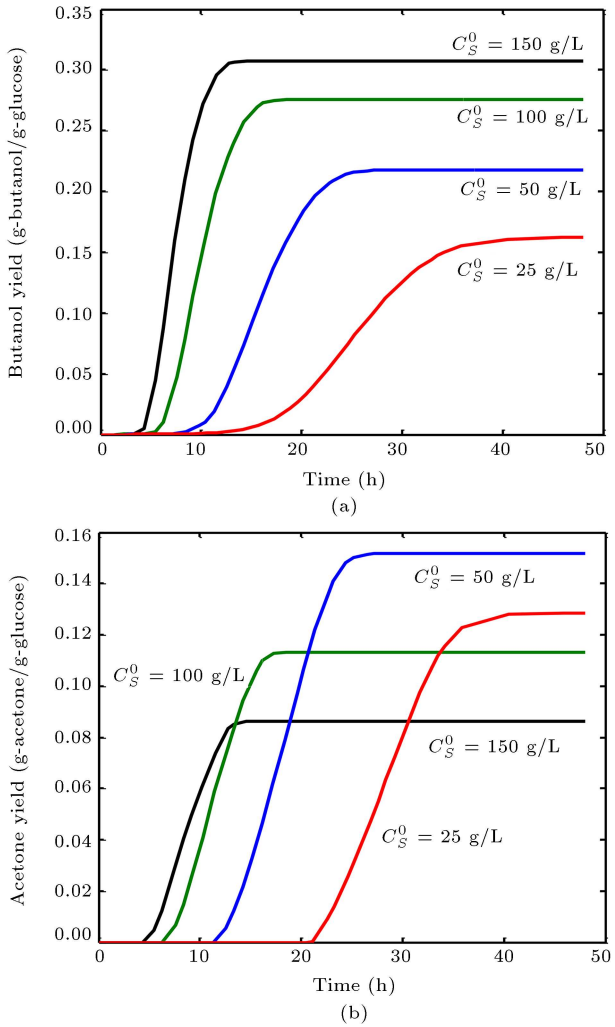

Figure 3. Effect of the initial concentration of substrate on the (a) butanol yield and (b) acetone yield at various operating times.

effect on the solvent yield and must stay on the list of optimization parameters.

Figure 4 represents the time variations of substrate conversion at the initial substrate concentrations of substrate 25, 50, 100, and 150 gL^{-1}. At a given initial concentration of glucose, the substrate conversion increases during the operating time and, then, reaches the stationary non-equilibrium state. Increasing the initial concentration of substrate shifts the S-shaped conversion profile to the left. This trend also occurs for the profile of solvent yield (see Figure 3). The system approaches the stationary non-equilibrium state after 40, 25, 18, and 15 h at C_S^0 = 25, 50, 100, and 150 gL^{-1}, respectively. Therefore, increasing the initial substrate concentration leads to a decrease in the time to the stationary non-equilibrium state. Finally, in the stationary non-equilibrium state, the substrate conversion reaches 1 for all initial concentrations of substrate.

The effect of the initial concentration of substrate

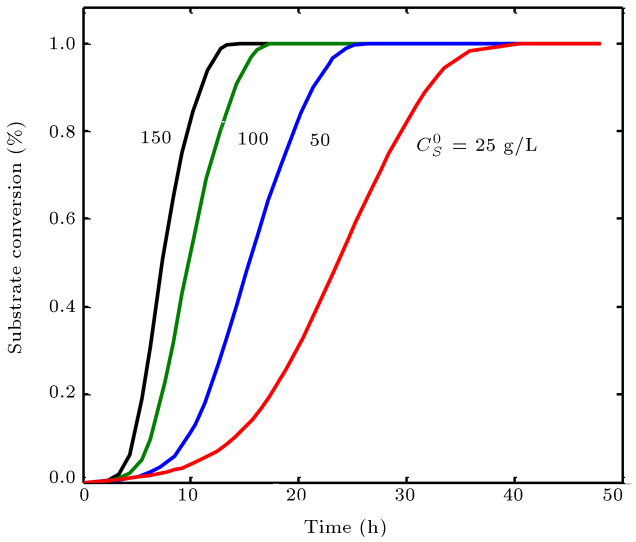

Figure 4. Effect of the initial concentration of substrate on the substrate conversion at the various operating times.

on the butanol and acetone productivity is illustrated in Figure 5(a) and (b), respectively. According to these figures, at a given initial concentration of substrate, the solvent productivity increases during the initial period of the operating time and a peak spot develops and, then, decreases monotonically. The butanol and acetone (also ethanol) productivity increases with the initial concentration of substrate from 25 to 150 gL^{-1}. Increasing the initial concentration of substrate causes the migration of the peak spot to the left in addition to causing an increase in the solvent productivity at this peak spot. At C_S^0 = 100 gL^{-1}, this peak spot occurs at the operating times of 13.31, 15.75, and 15.96 h for the butanol, acetone, and ethanol, respectively. Therefore, the operating time plays an important role in the solvent productivity. As the peak spots arise at different operating times for each solvent, a proper objective function (like f_2) must be defined to determine the optimal final operating time.

6.3. Bi-objective optimization results

With due attention to the subjects of Section 3.5.1 and the parametric sensitivity analysis performed in Section 6.2, the bi-objective optimization approach is used to find the optimal initial concentration of substrate and the final operating time to maximize simultaneously f_1 and f_2, subject to differential mass balance equations as the equality constraints. In order to optimize the ABE fermentation process, the MODE code is integrated with a set of ordinary differential equations (Eqs. (1) and (2)).

The objective function f_1 versus f_2 is plotted, as indicated in Figure 6. The curve in this figure is introduced as a Pareto set, and each point in the Pareto set corresponds to an optimal solution and certain values of decision variables. It is obvious that the

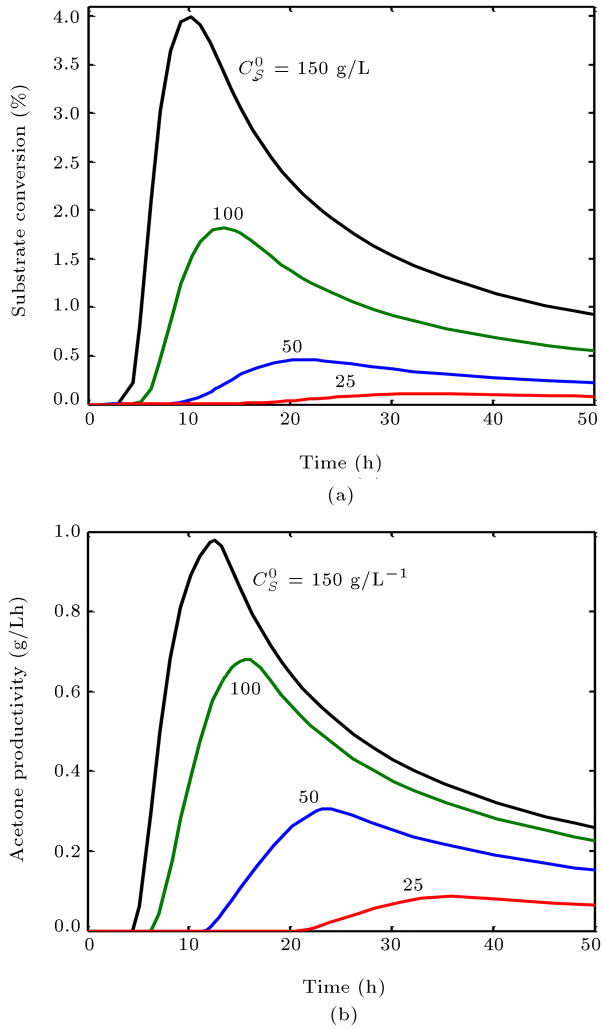

Figure 5. Effect of the initial concentration of substrate on the (a) butanol productivity and (b) acetone productivity at the various operating times.

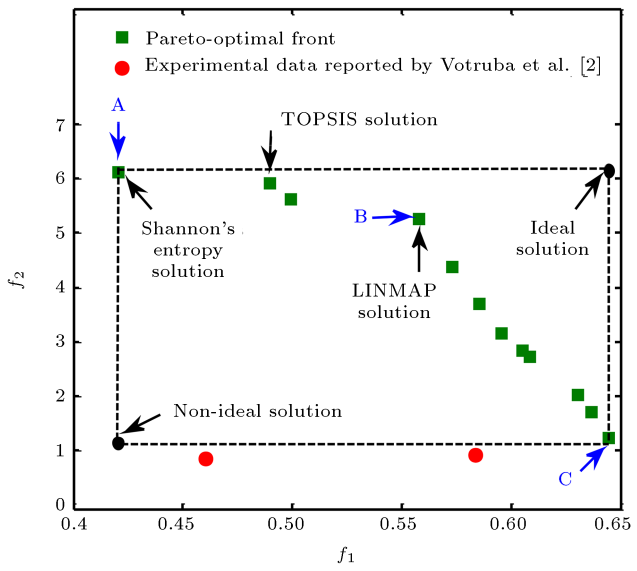

Figure 6. Pareto-optimal front in objective space.

suggested algorithm is able to generate a set of optimal solutions, not a unique solution. The obtained Pareto-optimal front is well distributed, which means that MODE performs well and is successful for this problem. Twelve non-dominated optimum points are obtained by the optimization algorithm. These points are equally good and have optimum values of both solvent yield and productivity. Shifting from one point to another leads to the enhancement of one objective function at the expense of the other. Three points A, B, and C are considered in this set. For instance, when shifting from point A to C, the objective function f_1 increases and f_2 decreases. The comparison of the experimental data and the optimum points in Figure 6 shows that the experimental data lie below the Pareto-optimal front, meaning that these data were not taken in optimal conditions. Votruba et al. [2] reported these experimental data at $C_S^0 = 50$ gL^{-1} and final fermentation time of 27 and 32 h. Table 4 represents the optimal values of the initial concentration of substrate and final operating time, as well as the objective functions (f_1 and f_2), for three chosen points, A, B, and C (shown in Figure 6). Point A shows the optimal operating conditions for the maximum solvent productivity, and point C illustrates the optimum operating conditions corresponding to the maximum solvent yield.

Table 4 verifies the fact that the two decision variables are in contrast in nature with respect to the objective functions. In order to determine the contrasting parameters and obtain a further understanding of the problem, the optimal decision variables are drawn against both objective functions, as shown in Figure 7(a)-(d). Figure 7(b) and (c) illustrate that C_S^0 and t_f have a strong opposing effect on f_1 and f_2, respectively. An increase in the initial concentration of substrate and the final operating time leads to a decrease in the solvent yield and solvent productivity, respectively. Figure 7(a) and (c) reveal that when the final operating time increases from lower bound to upper bound, f_1 increases from 0.42 to 0.64; however, f_2 decreases from 6.10 to 1.23. The optimum value of the initial concentration of glucose is found to vary from 54.72 to 145.36 gL^{-1}, whereas the optimal final operating time is found to change between 10 and 28.56 h.

Therefore, it should be taken into consideration that even the higher final operating time is favored for the solvent yield, which in turn decreases the solvent productivity. An opposing trend is observed for C_S^0. Increasing the initial concentration of substrate will lead to higher solvent productivity and, yet, lower solvent yield.

The Pareto-optimal front supplies a vast-ranging optimum set of operating conditions, where all points have the potential to give a final solution. The importance of the objective functions, design conditions, and demands of the user are the criteria for the selection

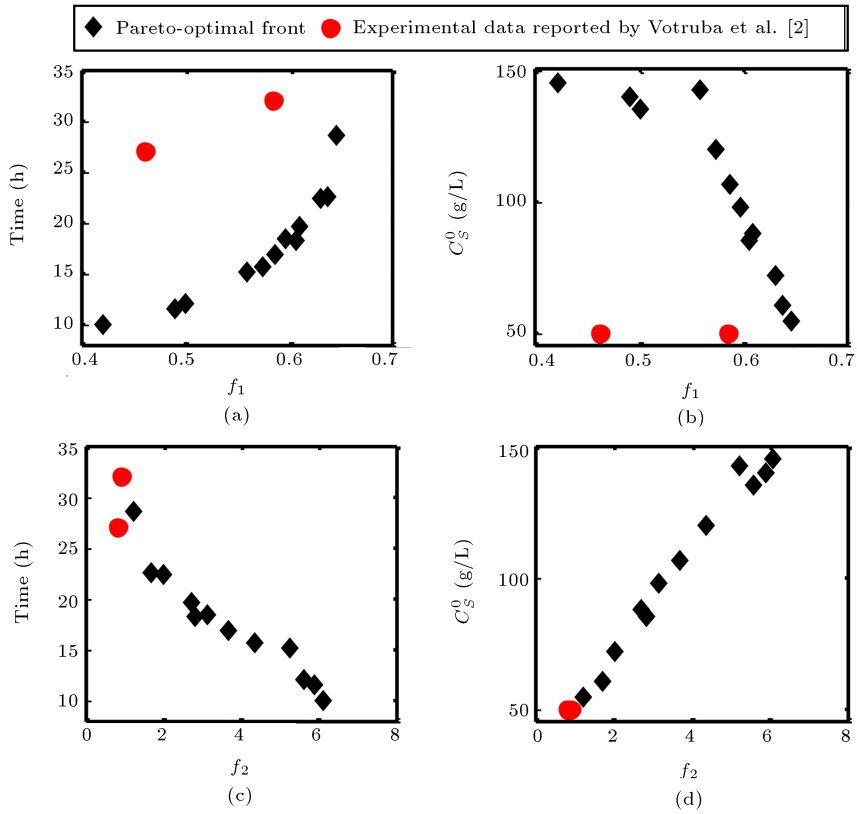

Figure 7. Values of decision variables corresponding to the points on a Pareto set in Figure 6 versus objective functions.

Table 4. Operating conditions, objective function, and deviation index corresponding to LINMAP, TOPSIS, and Shannon's solutions and points A, B, and C in Figure 6.

Optimization	Decision-making methods	Decision variables		Objective functions		Deviation index
		C_S^0 (gL^{-1})	t_f (h)	f_1	f_2 (gL^{-1}h^{-1})	
Bi-objective	Point A	145.36	10	0.420	6.109	0.245
	Point B	142.53	15.15	0.557	5.247	0.204
	Point C	54.72	28.56	0.644	1.234	0.754
	LINMAP	142.53	15.15	0.557	5.247	0.204
	TOPSIS	139.56	11.56	0.489	5.909	0.191
	Shannon's entropy	145.36	10	0.420	6.109	0.245
	Ideal solution	–	–	0.644	6.109	0
	Non-ideal solution	–	–	0.420	1.234	1
Single-objective based on maximum solvents yield		52.36	45.53	0.644	0.741	0.763
Single-objective based on maximum solvents productivity		150	11.16	0.451	6.579	0.198

of a proper solution from Pareto-optimal front. However, a suitable decision-making process is required for selecting the best solution from the Pareto set. In this study, the final optimal point has been chosen using three decision-making methods of TOPSIS, LINMAP, and Shannon's entropy. The final optimum solution reflected by TOPSIS, LINMAP, and Shannon's entropy decision-making approaches and the ideal and non-ideal solutions are represented in Figure 6. The optimal values of the two objective functions, the initial concentration of substrate, final operating time, and deviation index obtained through these decision-making approaches are listed in Table 4. The lowest value of deviation index describes the closeness of each point to the ideal solution and its distance from the non-ideal solution. According to the values of the deviation index, the optimum point obtained by TOPSIS with $DI = 0.191$ is more suitable than that found by LINMAP and Shannon's entropy approach with $DI = 0.204$ and 0.245, respectively. Therefore,

a combination of the bi-objective optimization results and the decision-making methods shows that the substrate initial concentration of 139.56 gL^{-1} and the final operating time of 11.56 h are the best feasible points for the ABE fermentation process. At this point, the solvent yields including $Y_A = 0.073$, $Y_B = 0.283$, $Y_E = 0.010$ and the solvent productivities including $P_A = 0.881$, $P_B = 3.415$, $P_E = 0.122$ g $L^{-1}h^{-1}$ are achieved.

The last two rows of Table 4 indicate the results of single-objective optimization based on maximum solvent yield and maximum solvent productivity, separately. Lower deviation indexes for the bi-objective optimization in comparison with the corresponding values for single-objective conclude that the results of bi-objective optimization are more favorable.

6.4. Economy-based optimization results

The economy-based optimization of the ABE fermentation process is carried out using the DE algorithm. From a profit function point of view, results show that the initial concentration of 150 gL^{-1} and the final operating time of 11.52 h are the most economical operating points, in which the solvent yields are $Y_A = 0.073$, $Y_B = 0.295$, $Y_E = 0.010$ and solvent productivities are $P_A = 0.957$, $P_B = 3.842$, $P_E = 0.135$ gL^{-1} h^{-1}. At this point, the profit value is US\$2.62 L^{-1} $year^{-1}$.

6.5. Comparison between TOPSIS solution and economy-based optimization

A comparison between the results of economy-based optimization and TOPSIS solution as an optimal point of bi-objective optimization is shown in Table 5. Although the amounts of solvent yield are almost the same in both optimizations, the amounts of solvent productivity in the economy-based optimization are more than those in TOPSIS solution. The final fermentation time in TOPSIS solution is nearly identical to that in economy-based optimization; however, the substrate consumption in TOPSIS solution is 7% lower than that in the economy-based optimization. In the last row of this table, the profit value of economy-based solution is 13% higher than that of TOPSIS solution. Hence, the optimal point obtained through the economy-based optimization is a more economical operating point compared with the TOPSIS solution.

Table 5. Comparison between TOPSIS solution and the economy-based optimization.

	TOPSIS solution	**Economy-based optimization**
C_S^0 (gL^{-1})	139.56	150
t_f (h)	11.56	11.52
Y_A	0.073	0.073
Y_B	0.283	0.295
Y_E	0.010	0.010
P_A ($gL^{-1}h^{-1}$)	0.881	0.957
P_B ($gL^{-1}h^{-1}$)	3.415	3.842
P_E ($gL^{-1}h^{-1}$)	0.122	0.135
Profit (US\$$L^{-1}$ $year^{-1}$)	2.319	2.62

7. Conclusion

This study investigated the bi-objective optimization and economy-based optimization of a batch ABE biological reactor by a dynamic mathematical model. The model was validated against the experimental data, as reported by Votruba et al. [2], and good agreement was obtained. The effect of the initial concentration of substrate on substrate conversion, solvent yield, and solvent productivity was investigated. The MODE algorithm, as an effective and robust optimization method, was used to specify the optimal operating conditions, namely initial concentration of substrate and final operating time of the process; in this regard, two objective functions were defined in terms of solvent yield and productivity. A Pareto optimal set was achieved, and a final optimum point was chosen through TOPSIS, LINMAP, and Shannon's entropy decision-making methods. The following key results are achieved:

- The butanol yield increased with the initial concentration of substrate; however, the acetone and ethanol yield firstly increased and, then, decreased;
- The maximum value of the solvent productivity could be increased by increasing the initial concentration of substrate; this maximum point occurred in a shorter operating time period;
- Based on the economy-based optimization, the most economical operating condition was found at an initial concentration of 150 gL^{-1} and the final operating time of 11.52 h;
- The best optimal point obtained by TOPSIS decision-making approach according to the lowest value of deviation index was achieved at an initial substrate concentration of 139.56 gL^{-1} and the final operating time of 11.56 h. However, the application of multi-objective optimization can considerably aid decision-maker in choosing any one of the optima from the Pareto set corresponding to his/her interest in order to maximize a specific objective.

Nomenclature

C	Concentration, g L^{-1}
DD_j	deviation degree of the jth objective function
DI	Deviation Index
F	Objective function

F	Non-dimensionalized objective function
K	Kinetic constant in the models
k_I	Inhibition constant
k_S	Saturation constant for substrate (glucose)
k_{AA}	Saturation constant for acetic acid
k_{BA}	Saturation constant for butyric acid
N	Cost, US\$kg^{-1}
P	Productivity, g L^{-1}h^{-1}
R	Rate of reaction, g L^{-1}h^{-1}
T	Time, h
t_c	Cleaning time in each cycle (= 2 h)
t_f	Final operating time (h)
W_j	Weight of jth objective function
Y	Yield
y	Marker of the physiological state of the culture

Greek letters

λ	Number of bacterial culture

Superscripts

0	Initial conditions

Subscripts

A	Acetone
AA	Acetic Acid
B	Butanol
BA	Butyric Acid
CO_2	Carbon dioxide
E	Ethanol
H_2	Hydrogen
S	Substrate (glucose)
X	Biomass

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