Chemical Engineering Research and Design 214 (2025) 39–53

Contents lists available at ScienceDirect

Chemical Engineering Research and Design

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

A comparative analysis of differential evolution and Boltzmann-based distribution algorithms with constraint handling techniques for distillation process optimization

R. Murrieta-Dueñas [a], J. Cortez-González [a], J.G. Segovia-Hernández [b,*], A. Hernández-Aguirre [c], R. Gutiérrez-Guerra [d], S. Hernández [b]

[a] Tecnológico Nacional de México/Campus Irapuato, División de Ingeniería Química, Silao-Irapuato km 12.5 El Copal, Irapuato, Gto 36821, Mexico
[b] Universidad de Guanajuato, Campus Guanajuato, Departamento de Ingeniería Química, Noria Alta s/n, Guanajuato, Gto 36050, Mexico
[c] Centro de Investigacion en Matematicas A.C., Departamento de Ciencias Computacionales, Callejón de Jalisco s/n, Mineral de Valenciana, Guanajuato, Gto 36240, Mexico
[d] Universidad Tecnológica de León, Campus I, Área de sustentabilidad para el desarrollo, Blvd. Universidad Tecnológica, 225,Col. San Carlos, León, Gto C.P. 37670, Mexico

ARTICLE INFO

Keywords:
DE
BUMDA
DE-BUMDA Comparison
Distillation systems optimization
DE-BUMDA Performance

ABSTRACT

Evolutionary algorithms, which emulate natural selection and species evolution, have long been applied to process optimization in chemical engineering. While these methods have demonstrated robustness to various optimization challenges, their computational requirements escalate with increasing case study complexity. This paper investigates the application of the Boltzmann Univariate Marginal Distribution Algorithm (BUMDA) as an optimization tool for distillation processes. BUMDA is a distribution estimation algorithm (EDA) based on the Boltzmann distribution, characterized by its alignment to the optimal value of the fitness function. The performance of BUMDA is benchmarked against Differential Evolution (DE), a widely adopted algorithm in chemical engineering optimization. Both algorithms are coupled with a self-adaptive constraint handling technique. The optimization objective is to minimise the total heat input in three different distillation systems while satisfying purity and recovery constraints. Results indicate that BUMDA outperforms DE, yielding superior solution quality, reduced computational complexity and lower computing time. Furthermore, BUMDA effectively avoids local minima entrapment. A statistical comparison of the algorithms using bootstrap test, confirms the enhanced performance of BUMDA over DE.

1. Introduction

In the realm of chemical engineering, optimization is a critical tool for designing systems that utilize resources efficiently, thereby minimizing environmental impacts. The complexity of chemical engineering problems stems from their highly nonlinear, multivariable nature, encompassing both discrete and continuous variables, and often bound by thermodynamic or design constraints. These challenges necessitate robust and efficient optimization tools to achieve feasible and optimal solutions [Kim and Wankat, 2004; Hu et al., 2022].

Distillation is among the most widely utilized separation processes in chemical engineering, playing a critical role in purifying multicomponent mixtures, especially within the chemical and petrochemical industries. As a highly energy-intensive operation, distillation accounts for a substantial portion of energy consumption in industrial processing, making energy optimization an essential focus within process design. Considerable research has therefore been devoted to improving the energy efficiency of distillation configurations, given that the optimal design of multicomponent distillation systems remains one of the most complex and challenging issues in process engineering.

To address these challenges, researchers have introduced innovative designs aimed at enhancing efficiency and reducing energy requirements. These designs include advanced configurations such as divided-wall columns, thermally coupled systems, and thermodynamically equivalent configurations. In addition, intensified operation concepts, such as the integration of reactive stages directly within

* Corresponding author.
E-mail address: gsegovia@ugto.mx (J.G. Segovia-Hernández).

https://doi.org/10.1016/j.cherd.2024.12.013
Received 22 August 2024; Received in revised form 17 November 2024; Accepted 5 December 2024
Available online 12 December 2024

distillation columns, have been proposed to further enhance energy performance (Weinfeld et al., 2018; Amminudin, et al., 2001; Petlyuk, 1965). Each of these advancements contributes to the development of new separation schemes that significantly reduce total process costs by lowering energy consumption.

Optimizing the efficiency of distillation processes not only achieves cost reductions but also results in substantial energy savings and environmental benefits, aligning with broader sustainability goals. The ongoing exploration of these advanced configurations underscores the importance of energy-efficient designs in achieving both economic and ecological benefits in chemical processing industries.

Early analyses of distillation synthesis and design were conducted by pioneers such as Siirola et al. (1971) and Lockhart (1947). These foundational studies highlighted the inherent challenges associated with distillation, setting the stage for subsequent advancements. In recent years, the focus has shifted towards reducing the energy consumption of distillation processes through optimization strategies. This shift is driven by the fact that distillation accounts for approximately 3 % of global energy consumption, underscoring the importance of developing more energy-efficient designs (Masoumi and Kadkhodaie, 2012).

To improve the performance of conventional and complex distillation schemes, both stochastic and deterministic optimization tools have been implemented. These distillation schemes are typically modeled using MESH (Material, Equilibrium, Summation, and Heat) equations, which are subject to constraints on purity and recovery for each component. These equations define the optimization problem as nonconvex, mixed-integer, highly nonlinear, multivariable, and constrained, making the optimization process particularly challenging.

Deterministic optimization strategies involve considering the distillation sequence as superstructures, which can be solved using methods such as mixed-integer linear programming (MILP), nonlinear programming (NLP), or reduced models (Andrecovich, Westerberg, 1985; Chen and Grossmann, 2017; Viswanathan, and Grossmann, 1993; Trespalacios and Grossmann, 2014; Bauer and Stichlmair, 1996; Yeomans and Grossmann, 2000; Segovia-Hernández et al., 2015). This approach requires strong mathematical formulations to simplify the rigorous models, and convergence is highly dependent on a good initial guess. Additionally, significant computing time is often necessary to achieve a solution, which can be a limiting factor in practical applications.

In contrast, stochastic algorithms can evaluate the objective function as a black-box model, allowing for the rigorous modeling of MESH equations to be maintained throughout the optimization process. This flexibility makes stochastic algorithms particularly attractive for complex, nonlinear problems. A diverse set of stochastic algorithms has been applied to the optimization of distillation columns. For instance, simulated annealing has been used for optimizing pressure swing distillation (PSD) to find the minimum total annual cost for azeotropic (Wang et al., 2016; Fulgueras et al., 2016; Fulgueras et al., 2018) and ternary mixtures (Zhu et al., 2016). Internally heat-integrated distillation column (HIDiC) schemes have been optimized using Genetic Algorithms (Yala et al., 2017) (GA) and combinations of GA with Particle Swarm Optimization (PSO). Self-adapting dynamic differential evolution (SADDE) has been applied to optimize distillation sequences for ternary systems (Cui et al., 2019), while surrogate models have been used for global optimization of both ideal and non-ideal distillation columns (Keßler et al., 2019). Particle Swarm Optimization (PSO) has been employed for the optimal design of dividing wall columns (Jia et al., 2017) (DWC) and for response surface optimization of separation processes (Weerachaipichasgul, et al., 2019). In the petroleum industry, ant colony algorithms (Udoeyop et al., 2018) and surrogate-aided models (Xue et al., 2019) have been used for optimizing oil production and other (Cortez-Gonzalez et al., 2012) processes.

The literature indicates that various stochastic algorithms have been employed in the optimization of separation systems, particularly in distillation configurations (Ochoa-Estopier et al., 2015; Sudibyo et al., 2015; Wang et al., 2012; Modla et al., 2010; Martins and Costa, 2010). A majority of these algorithms fall within the category of evolutionary algorithms. Evolutionary algorithms are systematic approaches to solving search and optimization problems that draw on principles of natural evolution, including competition-based selection of the fittest individuals, reproduction, and mutation to generate successive generations. Key examples of these bio-inspired stochastic methods, which computationally emulate evolutionary mechanisms, include Differential Evolution, Genetic Algorithm, Tabu Search, Bat Algorithm, and Ant Colony Algorithm (Cheng et al., 2009; Gutiérrez-Antonio et al., 2014; Li et al., 2015; Hanke and Li, 2000; Cardoso et al., 2000; García-Herreros et al., 2011; Modla and Lang, 2012; Cortez-Gonzalez et al., 2012).

In evolutionary algorithms, reproduction is typically the primary operator. However, in the case of Differential Evolution, mutation is the dominant operator, guiding the search space exploration to identify promising regions with optimal values of the fitness function (Srinivas and Rangaiah, 2007). These promising regions represent areas within the search space where the best fitness function values have been located, driving the optimization process toward high-quality solutions.

Despite their robustness and flexibility, stochastic algorithms often incur high computational costs due to the numerous function evaluations required to find an optimal solution. Among these, the differential evolution (DE) algorithm stands out for its efficiency in solving benchmark and fundamental chemical engineering problems (Srinivas and Rangaiah, 2007). Cortez-González et al. (2023) presented a comparative study of the Differential Evolution (DE) algorithm employing a weighted sum constraint-handling technique against a self-adaptive constraint-handling technique in the optimization of separation schemes. The results indicate that when a weighted sum constraint-handling approach is utilized, the computational complexity of DE increases substantially. Additionally, as the complexity of the separation scheme escalates, so does the computational effort required for optimization. While DE demonstrates efficiency across various case studies, its application to large-scale problems significantly amplifies computational demands, potentially limiting its practicality in such contexts.

Another class of stochastic algorithms, known as Estimation of Distribution Algorithms (EDAs), approximates the probability distribution of the population during the optimization process (Larrañaga and Lozano, 2012). EDAs aim to reach the optimal solution by constructing a probability model based on the best-performing subset of individuals in each generation. This subset is then used to generate or simulate the individuals of the subsequent generation, bypassing the need for traditional reproduction and mutation operators (Valdez et al., 2008).

Given these considerations, there is a clear need for robust stochastic algorithms that not only deliver high performance but also reduce computational time and numerical effort. Such advancements would enhance the practicality and accessibility of these algorithms across a broader range of chemical engineering applications, particularly in distillation process optimization.

One notable EDA within this category is the Boltzmann Univariate Marginal Distribution Algorithm (BUMDA), which is based on the Boltzmann distribution. This distribution steers the population toward the optimum, with the distinctive property that the maximum value of the Boltzmann distribution aligns with the highest fitness value of the objective function. BUMDA facilitates both exploration and intensification in the search space: high variance initiates the exploration process to identify promising regions, while reduced variance focuses intensification efforts within these regions. Each design variable in BUMDA is modeled by the Boltzmann distribution, creating a synergy with the normal distribution. The Boltzmann distribution indicates the optimal value of the design variable, while the normal distribution that best approximates the Boltzmann distribution is employed to generate new individuals for the next generation.

This study proposes a comparative analysis of the performance of the evolutionary algorithm DE and the Boltzmann-based EDA, BUMDA. Both algorithms are integrated with a self-adaptive constraint-handling technique to enhance search space exploration. Specifically, we have

selected DE and BUMDA for coupling with the constraint-handling technique introduced by Cortez-González et al. (2023). The comparison evaluates the algorithms based on computational effort, objective function quality, and the numerical precision of the best value identified by each algorithm. The study involves the optimization of several distillation configurations: a binary column, a four-component distillation train and an intensified column for quaternary mixture separation.

To rigorously evaluate the performance of both algorithms, statistical analysis using resampling with replacement was conducted. This approach provides a robust framework for comparing the efficiency and effectiveness of the algorithms under various scenarios. Additionally, a nonparametric hypothesis test called Bootstrap was performed to determine if there were significant differences in the solutions found by the two algorithms. The results of this comparative analysis aim to highlight the advantages and potential drawbacks of each algorithm, ultimately contributing to the development of more efficient and practical optimization tools for the chemical engineering community.

2. Optimization strategy

Distillation columns are pivotal in chemical engineering processes for separating components based on their boiling points. Enhancing the efficiency of these columns involves optimizing variables like feed location and reflux ratio while ensuring product purity and operational efficiency. Traditional optimization methods struggle with the nonlinear and multivariate nature of distillation column optimization. In recent years, stochastic optimization algorithms have emerged as powerful tools capable of effectively tackling such complex problems. The optimization of distillation columns presents a formidable challenge due to the inherent complexity arising from both discrete and continuous variables such as the number of stages, feed stage, and reflux ratio. Rigorous modeling of these columns necessitates thermodynamic models to accurately predict phase equilibrium, often characterized by highly nonlinear behavior. Consequently, optimizing distillation columns becomes a multivariate, non-convex, nonlinear problem constrained by thermodynamic and design limitations.

Differential Evolution (DE), introduced by Storn and Price in 1995, has garnered significant attention in the field of chemical engineering due to its versatility and robustness in optimizing complex separation schemes (Storn and Price, 1995; Storn and Price, 1997). DE is classified as a stochastic evolutionary algorithm that iteratively improves solutions using mutation and crossover operators. Unlike gradient-based methods, DE is particularly suited for non-differentiable, non-convex, and multi-modal optimization problems encountered in distillation column design.

DE initializes a population of individuals randomly within the search space defined by decision variables such as reflux ratio and stage efficiencies. Fig. 1 shows the DE pseudocode. At each iteration, termed as a generation, DE selects parents from the current population. Mutation, a key operator in DE, enhances diversity by perturbing selected individuals using a strategy involving differential vectors scaled by a mutation factor (F). This process generates trial solutions that are subsequently recombined with the parent solutions using a crossover rate (CR). Finally, the trial solutions replace parents if they exhibit superior fitness, thereby driving the population towards optimal solutions.

The effectiveness of DE lies in its ability to explore diverse regions of the search space while exploiting promising solutions to converge towards global optimal. This is crucial in distillation column optimization, where finding optimal operating conditions can significantly impact process efficiency and profitability.

DE has been extensively applied in various domains of chemical engineering, including distillation column design. Studies by Yerramsetty and Murty (2008), Preechakul and Kheawhom (2009), Peng and Cui (2015) have demonstrated DE's robust performance in optimizing distillation configurations under rigorous thermodynamic models. These investigations highlight DE's capability to handle complex decision spaces and nonlinear objective functions effectively.

2.1. BUMDA

The Boltzmann Univariate Marginal Distribution Algorithm (BUMDA) was developed following the establishment of principles for algorithms based on distribution estimates by Valdez et al. (2008). Initially, BUMDA was designed to solve unconstrained optimization problems in continuous variable search spaces.

BUMDA is based on the Boltzmann distribution, $P(x)$, a key characteristic of which is its implicit inclusion of the objective function. It depends on two parameters, β and Z, where z is the normalization parameter, represented in Eq. 1. This distribution can describe the trajectory of the objective function, as the mode of the Boltzmann distribution aligns with the optimum of the objective function. This ensures that the search always moves towards the optimum, even in the presence of clusters in infeasible regions during the optimization process. This feature sets the BUMDA apart from all other stochastic algorithms used

Generate random initial population Np
Evaluate initial population in objective function
Do
While (Stop criteria)
For $(j = 1; j \leq Np; j++$
Do
Generate 3 random integers $(r1, r2, r3) \in [1, Np]$ *with* $r1 \neq r2 \neq r3 \neq j$
Generate a random integer $i_{rand} \in (1, n)$
For each i_{rand}

$$v_{i,j,G+1} = \begin{cases} z_{i,r3,G} + F * \left(z_{i,r1,G} - z_{i,r2,G}\right) & if \ rand(0,1) < CR \\ z_{i,j,G} & Othrwise \end{cases}$$

end For
Evaluate $v_{i,j,G+1}$ *in objective function*
Replace $v_{i,j,G}$ *with* $v_{i,j,G+1}$ *if* $v_{i,j,G+1}$ *is better*
end For
end while

Fig. 1. Differential Evolution (DE) pseudocode.

in chemical engineering.

$$P(x) = \int_x \frac{e^{\beta f(x)}}{z} dx \quad (1)$$

Since the Boltzmann distribution requires an infinite population to find the solution, it is approximated by a normal distribution. The mean (μ) and variance (σ)are calculated from the population of generation *t-1*, to generate a curve $Q(x,N)$. This curve is used to minimize the distance between the normal distribution and the Boltzmann distribution using Eq. 2.

$$KL_{PQ} = \int_x P(x) \log \frac{Q(x)}{P(x)} dx \quad (2)$$

Eq. 2 represents the Kullback-Leibler divergence, KL_{PQ}, defined as the difference between the points of the normal distribution, $Q(x)$, and the Boltzmann distribution $P(x)$. As a univariate algorithm, each dimension requires a normal distribution. The BUMDA proposed by Valdez et al. (2013) was tested with benchmark functions and compared with algorithms based on distribution estimation through statistical analysis. The comparison included univariate algorithms such as BG-UMDA and multivariate algorithms such as EMNA-B, the Iterated Density Estimation Evolutionary Algorithm (IDEA), the Covariance Matrix Adaptation Evolution Strategy (CMA-ES), and the Scaled Variance Adaptive Correlation IDEA (CT-AVS-IDEA). The results demonstrated BUMDA as a powerful optimization tool excelling in its application niche. Test problems were used to compare the convergence, optimal approximation, and scalability of BUMDA with state-of-the-art Estimation of Distribution Algorithms (EDAs). The results provided evidence for BUMDA's competitiveness compared to multivariate algorithms.

Due to the advantages offered by BUMDA, it was chosen for the optimization of distillation systems in chemical engineering. The optimization of distillation columns is a constrained problem with both continuous and discrete variables, and its search space is multimodal and non-convex. These characteristics complicate finding the feasible region and increase the likelihood of falling into a local optimum. Currently, mechanisms coupled to stochastic optimization algorithms are necessary to enhance their performance. Fig. 2 details the modifications and implementation of the BUMDA to optimize distillation systems.

The first modification to the BUMDA was to extend its handling of dimensions in continuous and discrete spaces. The individuals of the first population are generated from a normal distribution bounded between the upper and lower limits of each variable. Each individual is evaluated by the objective function. The best individual minimizes the objective function and satisfies the constraints of the optimization problem. The population of generation t is ordered from fittest to least fit, and the best fraction of the population is selected to calculate the mean and variance. These parameters are used to generate the $t + 1$. The selected fraction can vary between 1/5 and 2/3; this paper determined through tuning that 1/3 is optimal for the optimization of distillation systems. Elitism is built into the BUMDA to avoid premature convergence, extend exploration, and enhance search efficiency.

During the optimization process, the mean and variance are determined at each generation. The variance represents the variability of the objective function relative to the population mean. A small variance indicates that the algorithm has converged to the best value found so far, prompting the intensification process. To improve exploration, variance re-initialization has been proposed. This mechanism allows the search to restart within the search space while retaining the best individual found up to that point. It enables both exploration of the search space and intensification in feasible zones during the optimization process. The main advantage of variance re-initialization is BUMDA's ability to avoid local optima. This process is repeated until the stopping criterion is met.

Recent research has positioned BUMDA as a competitor to Differential Evolution (DE) in optimizing distillation schemes. BUMDA leverages Boltzmann distribution principles to enhance exploration and exploitation capabilities, particularly in escaping local optima. One notable feature of BUMDA is its self-adaptive constraint handling technique, which dynamically adjusts solution feasibility during the optimization process.

BUMDA introduces a novel mechanism for handling constraints based on the Boltzmann distribution, enabling effective exploration of the solution space. By integrating a re-initialization strategy, BUMDA mitigates the risk of premature convergence and enhances the algorithm's ability to discover globally optimal solutions. This feature is particularly advantageous in distillation column optimization, where the presence of multiple local optima poses a significant challenge to traditional optimization techniques.

A comparative study between DE and BUMDA in distillation column optimization highlights their respective strengths and weaknesses. DE excels in scenarios requiring rapid convergence to near-optimal solutions, leveraging efficient mutation and crossover operators. In contrast, BUMDA's emphasis on exploration through Boltzmann-based sampling makes it resilient against premature convergence, improving its ability to locate global optima in complex, multimodal landscapes.

To illustrate the application of DE and BUMDA in distillation column optimization, consider three case studies involving the separation of a binary mixture, a distillation train for separating four components, and an intensified column for purifying a quaternary mixture. The distillation column model is described by the MESH equations (Material balance, Equilibrium relations, Summation equations, and Heat balance). The objective is to minimize the total heat duty, subject to constraints on product purity and recovery. The optimization variables include the number of stages, feed stage location, and reflux ratio. The thermodynamic properties are modeled using the Chao-Seader model to predict phase equilibrium.

The DE is implemented with a population size of 50, a scaling factor F= 0.8, and a crossover rate CR= 0.9. The BUMDA is implemented with a population size of 60, a selection parameter of 1/3, and a variance re-initialization threshold of 0.001. The optimization runs for 500 generations, and the results are compared in terms of heat duty, convergence behavior, and computational efficiency.

Sensitivity analysis indicates that the performance of both algorithms is influenced by the choice of algorithm parameters. For DE, the scaling factor F and crossover rate CR significantly impact convergence speed and solution quality. For BUMDA, the Boltzmann distribution parameter and variance re-initialization threshold are critical for maintaining diversity and avoiding premature convergence. This paper compares two evolutionary algorithms: Differential Evolution (DE) and the Boltzmann Univariate Marginal Distribution Algorithm (BUMDA) with a self-adaptive constraints handling technique, applied to the optimization of distillation schemes using a rigorous model (MESH equations). The BUMDA, based on the Boltzmann distribution, is not widely used in chemical engineering but is capable of escaping local optima and finding feasible zones due to the incorporated variance re-initialization mechanism.

2.2. Constraints handling technique

The case studies in this work involve both equality and inequality constraints, necessitating a robust constraint-handling technique. Fig. 2 illustrates the pseudo code for the constraint-handling technique implemented within the BUMDA, which is similarly applied to the DE. The technique begins by assessing the feasibility of an individual, rejecting infeasible ones through a "death penalty." The fitness function is penalized based on the degree of constraint violation, which is proportional to the violation magnitude and the deviation from the target purity or recovery for each component. Additionally, a dynamic threshold ε is introduced, converting an equality constraint into an inequality constraint. This threshold ε is halved once the entire

1. Parameters of algorithm and stop criteria

$n_{sample} \leftarrow 30$
$v_{min} \leftarrow 0.001$
$n_{select} = 1/3$

2. To generate the initial uniform population P_0 for $t = 0$

- Test the individual's feasibility

$If\ N_F > N_T$
$N_F = N_F - |N_T - N_F|$
$End\ if$

- Verify the individual's feasibility

$If\ RR \leq 0$
$RR = random()$
$End\ if$

- Verify configuration

$If\ N_F > N_{s1}$
$f(z_i, config1)$
$else$
$f(z_i, config2)$
$End\ if$

a) Evaluate the population

a. $f(z_i) \leftarrow$ AspenOne

b) Penalize the population

- Constraints by purities

$If\ purity < setpoint$
$w_i \leftarrow Selfadaptive\ handling\ technique$
$f(z_i) = f(z_i) + w_i * f(z_i)$
$End\ if$

- Constraints by recoveries

$If\ recovery < setpoint$
$w_i \leftarrow Selfadaptive\ handling\ technique$
$f(z_i) = f(z_i) + w_i * f(z_i)$
$End\ if$

c) Ranking-truncate of population

Sort fitness function $f(z_i)$

Truncate population

d) Calculate the approximation for μ and the v using the selected set n_{select}

$\mu = \frac{\sum_{i=1}^{nselect} x_i\ \bar{g}(x_i)}{\sum_{i=1}^{nselect} \bar{g}(x_i)}$	$v = \frac{\sum_{i=1}^{nselect} \bar{g}(x_i)\ (x_i - \mu)^2}{\sum_{i=1}^{nselect} \bar{g}(x_i)}$

where: $\bar{g}(x_i) = g(x) - g(x_{nselect}) + 1$

a) Generate the individuals of the new model $Q(x, t)$

3. For $i = 1\ to\ NEF_{max}$

$t \leftarrow t + 1$

b) Evaluate the population

$f(z_i) \leftarrow$ AspenOne

c) Penalize the population

- Constraints by purities

$If\ purity < setpoint$
$w_i \leftarrow Selfadaptive\ handling\ technique$
$f(z_i) = f(z_i) + w_i * f(z_i)$
$End\ if$

- Constraints by recoveries

$If\ recovery < setpoint$
$w_i \leftarrow Selfadaptive\ handling\ technique$
$f(z_i) = f(z_i) + w_i * f(z_i)$
$End\ if$

d) Ranking-truncate of population

Sort fitness function $f(z_i)$

Truncate population

e) Calculate μ and v using the selected set n_{select}

$\mu = \frac{\sum_{i=1}^{nselect} x_i\ \bar{g}(x_i)}{\sum_{i=1}^{nselect} \bar{g}(x_i)}$	$v = \frac{\sum_{i=1}^{nselect} \bar{g}(x_i)\ (x_i - \mu)^2}{\sum_{i=1}^{nselect} \bar{g}(x_i)}$

where: $\bar{g}(x_i) = g(x) - g(x_{nselect}) + 1$

f) Variance Reset

$If\ v_{t,j} < v_{min}$
$v_{t,j} = v_{max}$
$End\ if$

g) Generate the individuals of the new model $Q(x, t)$

h) Insert the elite individual

Fig. 2. Pseudocode of the BUMDA for the optimization of distillation systems.

population satisfies all constraints. Static penalties are also incorporated, where the penalty coefficient increases with the level of violation. Another penalty factor increases when the total number of stages, as defined by the user, is exceeded. This maximum stage number is determined according to heuristic design rules dependent on the mixture types. This procedure continues until the number of function evaluations reaches the maximum allowed. This constraint-handling technique is detailed by Cortez-Gonzalez et al. (2023). In this paper, the purities of each component are within the range defined by the dynamic threshold of the restriction handling technique. In each case study, the dynamic threshold reached was 0.001, so the purity fluctuates in that proportion with respect to the desired purity value for each component.

2.3. Optimization process

The optimization process starts with the master program (either the DE or BUMDA) generating the initial population. The design variables are sent to Excel, where their feasibility is verified, and these variables are then used to call Aspen One for evaluating the fitness function. The evaluated fitness value is returned to Excel to compute the constraints, and the resultant value is sent to Matlab, where population sorting occurs. This information is used to generate the next population. This iterative process continues until the stopping criteria, defined by the maximum number of function evaluations, is reached.

3. Cases studies

In chemical engineering, the modeling of distillation processes relies heavily on MESH equations—an intricate system of nonlinear and nonconvex equations that describe Material balance, Equilibrium relations, Summation equations, and Heat balance for each stage within a distillation column. These equations are interdependent, making the MESH model highly complex and computationally demanding. Solving MESH equations requires robust algorithms capable of handling the inherent mathematical challenges associated with nonlinearity, nonconvexity, and high dimensionality, as even small-scale systems can demand significant computational resources.

This study examines three distinct case scenarios: a binary distillation column, a distillation train, and a quaternary distillation column. In each case, heat duty is selected as the objective function for evaluating and comparing the performance of the optimization algorithms under consideration. The heat duty, which represents the energy required by the distillation system to achieve the desired separation of components, is a crucial metric for process efficiency. Optimizing this value can lead to significant energy savings and operational cost reductions, which are essential in energy-intensive distillation processes.

By focusing on heat duty, the study aims to gauge the ability of each optimization algorithm to navigate the MESH model's complex solution space effectively. Specifically, the comparison of heat duty values across different optimization methods provides insights into each algorithm's capacity to locate feasible regions, avoid entrapment in local optima, and minimize computational effort while achieving an optimal solution. Because heat duty is independent of other design variables, it serves as an unambiguous measure of each optimizer's effectiveness, allowing for a clear assessment of its performance without interference from secondary variables.

Overall, this study's findings underscore the need for advanced algorithms in distillation process optimization, where achieving optimal separation outcomes through complex MESH modeling can have substantial impacts on both energy consumption and environmental sustainability in chemical processing.

Case 1. *Binary distillation column*

A binary distillation column separates a mixture into two products. The simplest sequence is shown in Fig. 3, where a feed stream enters the column, separating two adjacent components into top (light component) and bottom (heavy component) products. The column design considers the total number of stages, the reflux ratio, and the feed stage, aiming to minimize energy consumption. Although the reboiler duty energy is not an optimization variable, it is crucial for the optimal design for a given mixture and composition.

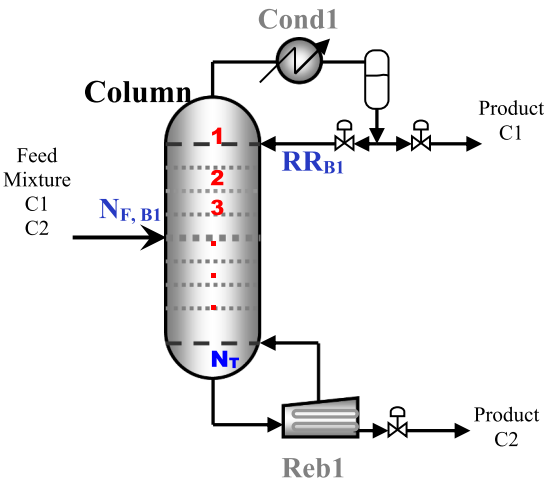


Fig. 3. Distillation column to split a binary mixture.

This study uses a binary mixture of butane and hexane with an equimolar composition. The relative volatilities of the adjacent components indicate that is easy separation is performed between n-butane, A, and n-hexane, B. The Chao-Seader thermodynamic model is used, with a feed flowrate of 100 kmol/h at 1 atm. The problem is defined as follows:

Find vector

$$Z = (NT, NF, RR) \tag{3}$$

To minimize fitness function

$$Q = f(Z) \tag{4}$$

Subject to constraint function

$$\begin{aligned} h_{1j}(Z) &= x^{\text{pur}}_{\text{target}} j = 1, \ldots, M_{\text{constraints}} \\ h_{2j}(Z) &= x^{\text{rec}}_{\text{target}} j = 1, \ldots, M_{\text{constraints}} \end{aligned} \tag{5}$$

and subject to boundary constraints

$$\begin{aligned} & z_i^{(L)} \le z_i \le z_i^{U} i = 1, \ldots, D \\ & 2 < NF \le NT \end{aligned} \tag{6}$$

Where: NT, NF, RR are total stages, feed stage and reflux ratio of the column respectively. In this problem the goal is to minimize the amount of energy in the reboiler, Q. The individual is represented by Z and D represents the number of variables or dimensions of the optimization problem. The upper and lower bounds correspond to $z_i^{(U)}$ and $z_i^{(L)}$, respectively. The Eq. 4 is subject to the set of constraints represented in Eqs. 5–6; they are handled as inequality constraints establishing a small deviation (tolerance) around the target defined, $x^{pur}_{\text{target}} = 0.99$ and $x^{rec}_{\text{target}} = 0.99$, that corresponding to the desired purity and recovery for each component. In a binary column, there exist four constraints; two of them impose by the purities and the others for the purities of each component. The equality constraints are treat as inequality constraints defining a threshold (ε) that relaxes the fitness function penalization in early generations, however the penalization becomes during optimization process (Eq. 7).

For instance, the equality constraint:

$$h_j(z) - k_j = 0 \quad \text{istreatedas}: \quad \left|\left(h_j(z) - k_j\right)\right| \le \varepsilon \tag{7}$$

Where k is the x_i^{pur} or x_i^{rec} for each component.

Thus, the constraint is evaluate to true when $\left(h_j(z) - k_j\right)$ is inside the interval$[-\varepsilon, +\varepsilon]$.

Last constraint (Eq. 7) is derive from the sequence design, because of the feed stage must be inside the range of the total stages of the column.

Results

Table 1 shows the best five individuals of each algorithm according to the best fitness function value, all meeting the constraints. For the DE, the best individual has a reflux ratio of 1.036, with 9 total stages and the feed introduced at stage 3, requiring 2.768 GW/year to split the mixture. Although individuals 3 and 4 have fewer total stages, their reboiler duty and reflux ratio are approximately doubled. The worst individual requires three times the total reboiler duty of the best due to a reflux ratio of 5.258, despite only a one-stage difference in total stages. All five individuals meet all constraints.

For BUMDA, the best individual demands 2.623 GW/year of heat duty with a design of 7 total stages, feeding at stage 4, and a reflux ratio of 0.896. The feed stage remains constant at 4 in all five individuals, with four individuals having 7 stages and one having 8. The best fitness function value of 2.623 GW/year compared to the worst 2.919 GW/year shows a slight variation due to a change in the reflux ratio from 0.896 to 1.171. All constraints are satisfied in all five individuals.

Case 2. *Distillation train*

A distillation train separates a multicomponent mixture into two adjacent components in each column, with the number of columns corresponding to n−1 for an n component mixture. For a four-component mixture (C1, C2, C3, C4), the first column separates the most volatile component (C1) at the top, with the rest at the bottom. The second column separates C2, and the final column separates C3 and C4. Fig. 4 illustrates the distillation train for a multicomponent mixture.

The mixture of four linear aliphatic hydrocarbons (C4-C6, C8) has a feed flow rate of 100 kmol/h, composed of 0.05, 0.45, 0.45, and 0.05 for n-butane, n-pentane, n-hexane, and n-octane, with purities 0.987, 0.98, 0.98 y 0.986, respectively. The mixture in our analysis is a mixture of hydrocarbons; the intermediate components, B and C, are of normal chain, and the light, A, and heavy, D. The feed composition contains a high concentration of the two intermediate components (90 %). The relative volatilities of the adjacent components indicate that the harder separation is performed between n-pentane, B, and n-hexane, C; the easiest cut is the light and heavy components: n-butane, A, and n-octane, D. The Chao-Seader model is used for the equilibrium liquid-vapor. Mathematically, the optimization problem is described by the 8–11 equations.

Find vector

$$Z = (NT_{B1}, NF_{B1}, NT_{B2}, NF_{B2}, NT_{B3}, NF_{B3}, RR_{B1}, RR_{B2}, RR_{B3}) \tag{8}$$

Table 1
Best five individuals obtained by DE and BUMDA Algorithms, Case 1.

Algorithm	Exp	Design variables			Fitness function
		N_T	N_F	RR	Q (GW/year)
DE	**Best**	**9**	**3**	**1.036**	**2.769**
	E1	8	6	1.234	2.992
	E2	6	4	2.686	4.588
	E3	6	3	2.868	4.787
	E4	10	3	5.258	7.288
BUMDA	**Best**	**7**	**4**	**0.896**	**2.624**
	E1	7	4	0.994	2.73
	E2	8	4	1.041	2.769
	E3	7	4	1.064	2.805
	E4	7	4	1.171	2.92

To minimize fitness function

$$Q = f(Z) \tag{9}$$

Subject to constraint function

$$g_{1j}(Z) = x_{\text{target}}^{\text{pur}} \quad j = 1, \ldots, M_{\text{constraints}}$$
$$g_{2j}(Z) = x_{\text{target}}^{\text{rec}} \quad j = 1, \ldots, M_{\text{constraints}} \tag{10}$$

and subject to boundary constraints

$$z_i^{(L)} \le z_i \le z_i^U i = 1, \ldots, D$$
$$2 < NF_{Bl} \le NT_{Bl} l = 1, \ldots, B_{columns} \tag{11}$$

In the optimization of distillation train the objective is find a vector Z variables (Eq. 8) that minimize the total heat duty, Q (Eq. 9). This vector is: the total stage number (NT), feed stage number (NF) and reflux ratio (RR), of each column (B). In the vector Z, NT and NF are discrete variables and RR is continuous variable. In this model optimization, the distillation train is constraint (Eq. 10) by to purity, $x_{\text{target}}^{\text{pur}}$ and the recovery, $x_{\text{target}}^{\text{rec}}$, of each component $N_{\text{components}}$. In addition, NF should always be less than NT and each dimension, z_i are between lower, z_i^L and upper z_i^U boundaries (Eq. 11).

Results

Table 2 presents the five best solutions obtained by the DE and BUMDA algorithms. For the DE, design variables vary significantly, with a 3 GW/year difference between the best and worst fitness function values. The reflux ratio values are similar across the three columns, with column 1 having a minimum value of approximately 14. In all designs, the total stages number exceeds 35 in at least one column. These individuals meet all constraints within the threshold value.

For the BUMDA, the worst fitness function value differs from the best by 2.350 GW/year, with the best at 22.849 GW/year. All columns in the five designs have fewer than 15 total stages. The feed stages are between 7 and 14, while the reflux ratio varies between 2.875 and 5.102.

Case 3. *Optimization of a quaternary mixture in a single column*

In this case, the goal is to separate a multicomponent mixture using the intensified sequences propose by Errico et al. (2009), who supposes that these configurations can reduce the energy consumption in relation with the conventional sequences (i.e. distillation train).

The intensified sequences (Fig. 5) have a feed stream and four out streams. The light component (C1) is obtained in the top column, the intermediate components (C2 and C3) are withdrawer in the side streams; while that the heavy component (C4) is removed in the bottom column. The intensified sequences are subject to several design conditions, such that the out stages of side streams must not be equal each other, neither with the feed stream stage.

These intensified sequences have three configurations possible (Fig. 5). The several configurations sequences, in this paper are named topologies. In the first configuration the feed stage is above the side streams; in the second topology the feed stage is between the side streams; and in the last configuration the feed stream is below the side streams. The main aim in these configurations is reduce the heat duty to achieve separation, however it depends of the design variables, such as total stages number (NT), feed stages (NF), location of the side streams stages (NS_1 and NS_2) and reflux ratio (RR).

The case study examined in this sequence intensified is the separation aliphatic chain hydrocarbon mixture (n-butane, n-pentane, n-hexane and n, octane) whose feed is made 0.30, 0.40, 0.25 and 0.05, respectability. As design targets, it is required that the four components achieve a recovery specification of 98 %; also, is required a purity of 98.7 % for the light component, 98.0 % for the intermediate components and 98.6 % for the heavy component.

The mixture in our analysis is another mixture of hydrocarbons; the light, A, intermediates, B and C, and the heavy component D, are of normal chain. The feed composition contains a concentration of the light

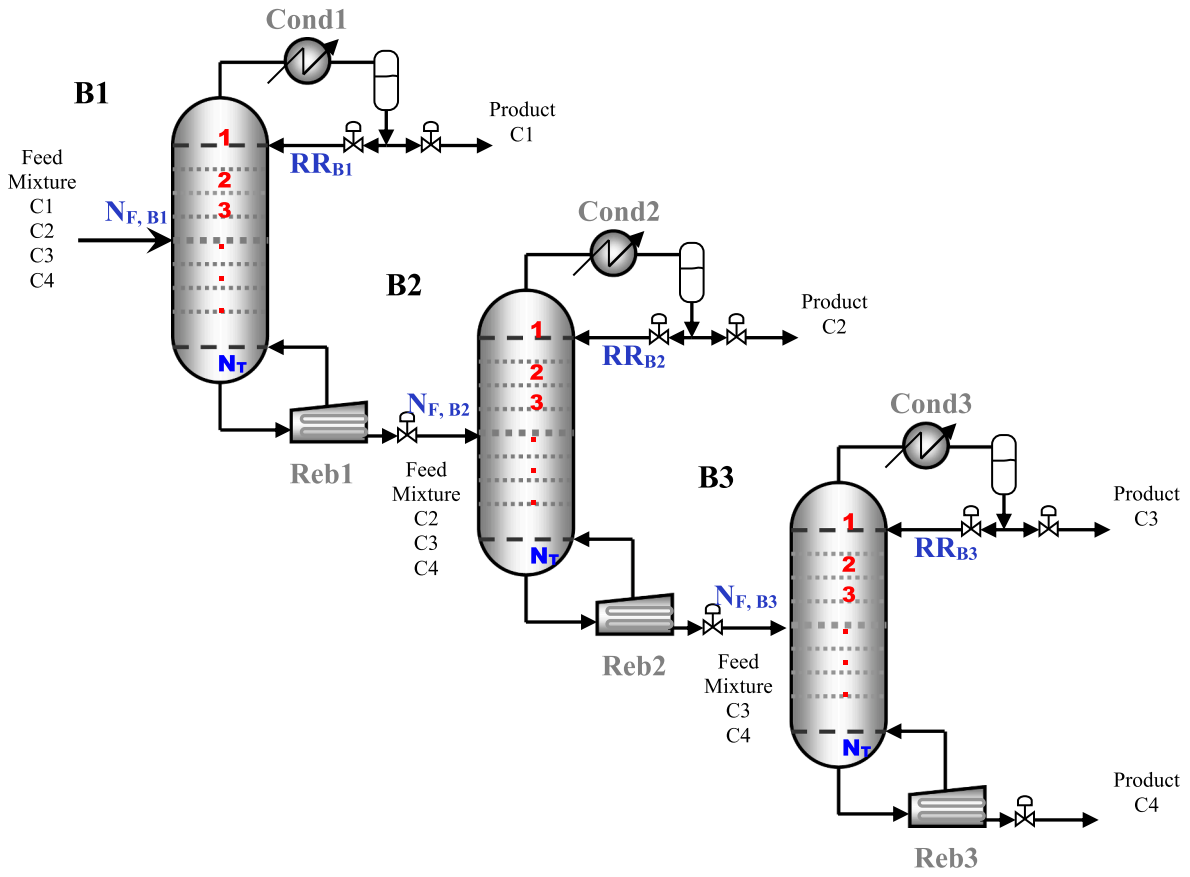


Fig. 4. Flowsheet of distillation train to split a four components mixture.

Table 2
The five Best individuals of the DE, distillation train, Case 2.

Algorithm	Exp	B1			B2			B3			Fitness function
		NT	*NF*	*RR*	*NT*	*NF*	*RR*	*NT*	*NF*	*RR*	Q (GW/year)
DE	**Best**	**18**	**11**	**20**	**34**	**21**	**3.946**	**30**	**19**	**1.482**	**9.426**
	E1	41	12	14.418	47	27	4.634	35	28	2.135	10.48
	E2	32	11	16.954	38	5	5.106	38	12	1.939	10.988
	E3	44	14	16.881	27	17	3.229	15	7	3.988	11.511
	E4	42	25	17.449	36	12	5.053	21	5	2.798	12.031
BUMDA	**Best**	**26**	**10**	**14.728**	**28**	**17**	**2**	**17**	**9**	**1.697**	**7.153**
	E1	23	10	14.949	24	15	2.812	19	12	1.629	7.962
	E2	27	16	14.411	30	7	2.411	16	10	2.311	8.348
	E3	24	10	14.765	17	10	3.133	20	13	1.8	8.519
	E4	23	12	15	16	11	4.004	15	7	1.8	9.500

component of 30 % (the second more abundant) and the heavy component of 5 % (the less abundant). The relative volatilities indicate that the separations are in general easy. In this case, the easiest cut is among n-hexane (C)/n-octane (D); the less easy includes n-pentane (B), and n-hexane (C).

In this case, the objective of the optimization is to minimize the total reboiler duty (Q) in the column, as shown in the adaptation function. The optimization problem is described by 12–15 equations.

Find vector

$$Z = (NT, NF, NS_1, NS_2, RR, \text{topology}) \tag{12}$$

To minimize fitness function

$$Q = f(Z) \tag{13}$$

Subject to constraint function

$$\begin{aligned} g_{1j}(Z) &= x_{\text{target}}^{\text{pur}} \quad j = 1, \ldots, M_{\text{constraints}} \\ g_{2j}(Z) &= x_{\text{target}}^{\text{rec}} \quad j = 1, \ldots, M_{\text{constraints}} \end{aligned} \tag{14}$$

and subject to boundary constraints

$$\begin{aligned} & z_i^{(L)} \le z_i \le z_i^{(U)} \qquad i = 1, 2 \ldots D \\ & 2 < NF \le NT \\ & NS_1, NS_2 < NT \\ & NF \ne NS_1 \ne NS_2 \end{aligned} \tag{15}$$

Where: *NT*is the total number of stages; *NF*is the feeding stage; NS_1 and NS_2 they are stages of extraction of the lateral currents and *RR* is the reflux ratio. The problem is having five design variables, of which four are discrete. In this problem, one more design variable was add, which is the optimal configuration (topology) to perform the separation, considering that for this case study there are three options. The topology

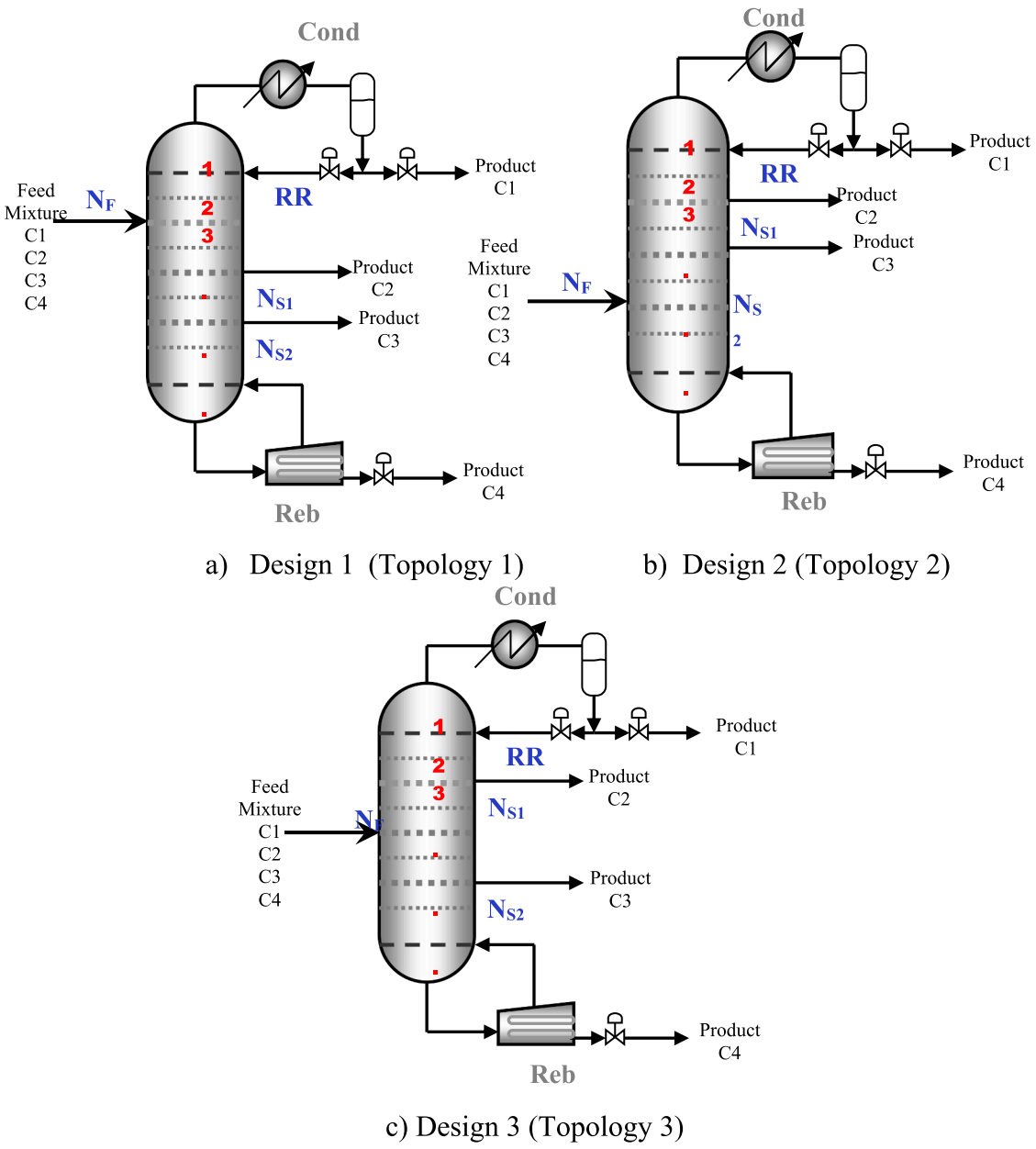


Fig. 5. Flowsheet of intensified sequences to split a four components mixture.

of the designs varies according to the position of the feed and the lateral currents. The authors define topology as the configuration that each distillation system can have.

Despite knowing a priori that this design is highly inflexible, it allows exploring the performance and versatility of the algorithm, since it requires handling two different thermodynamic constraints given by the feed stages and the lateral output currents. In this thermodynamic constraint, it is established that none of the currents must have at least 1 stage difference between them. While all these currents must be less than the total number of stages. Under this criterion, the algorithm evaluated the performance of three different configurations and throughout the optimization decided which was the best design.

Results

In Table 3, a more detailed comparative study is made about the best and worst value obtained by BUMDA respect to the heat duty, against the best design of DE. We can see that the best design obtained with the BUMDA has 3 GW/year below best designs of the DE. Likewise, although the heat duty does not represent a great difference, the BUMDA was able

Table 3
Comparative performance of best individuals obtained by DE and BUMDA algorithms, Case 3.

Algorithm	Exp	Design variables					Fitness function
		NT	NF	NS1	NS2	RR	Q (GW/year)
DE	**Best**	**68**	**36**	**23**	**52**	**70.232**	**39.861**
	E1	73	49	18	59	70.632	40.083
	E2	73	38	23	57	70.502	40.083
	E3	68	36	23	56	71.119	40.353
	E4	69	40	24	55	71.667	40.649
BUMDA	**Best**	**58**	**37**	**21**	**50**	**64.105**	**36.498**
	E1	71	37	24	49	64.123	36.502
	E2	71	37	25	54	64.747	36.843
	E3	58	40	21	49	65.679	37.365
	E4	62	32	21	42	65.870	37.462

to find a design able to reduce into more than 30 % the size of the column. For its part, with respect to the topology's optimization of the intensified sequence, it is possible to see that both optimizers agreed that the best configuration is one where the feed is located between the side streams. The location of the feed stage is in the range of 37–40 stages, while the side outputs of the best designs on both algorithms have similar or even identical values (Side 1). The reflux ratio value found varies in four units; however, this difference directly affects the amount of energy required. Now, taking into account the purities obtained, it must be emphasized that designs of the BUMDA are closer to the target values established by the problem, reason enough to say that the design is suitable to carry out the separation.

The comparative analysis of DE and BUMDA algorithms for optimizing distillation processes reveals that both algorithms can effectively find optimal solutions that meet all constraints. The BUMDA consistently produces solutions with lower energy consumption and fewer total stages compared to the DE. This study demonstrates the feasibility and efficiency of employing advanced evolutionary algorithms for optimizing complex distillation processes in the chemical industry. The BUMDA, with its ability to maintain diversity in the population and exploit the search space effectively, shows promise for broader applications in process optimization.

4. Discussion of results

In this paper is presents a comparison of the DE vs BUMDA. The two algorithms are tested to optimize three problems: the binary column, distillation train and a single column to separate four components. In two cases the stop criteria is the total number function evaluations. Besides, performing a comparison of statistical parameters with the bootstrap function.

The simulations were realize with a PC computer with i7 processor core, 16 GB of RAM and clock frequency at 2.8 GHz. The DE parameters using in all cases were $CR= 0.8$ and $F= 0.75$, and 100 individuals pear generations and 20,000 total function evaluations. For BUMDA use 60 individuals per generation with a total 3000 function evaluation and the parameter of truncate population is 1/3. In this paper is presents a comparison of the DE vs BUMDA. The two algorithms are tested to optimize three problems: the binary column, distillation train and a single column to separate four components. In two cases the stop criteria is the total number function evaluations. Besides, performing a comparison of statistical parameters with the bootstrap function.

The simulations were realize with a PC computer with i7 processor core, 16 GB of RAM and clock frequency at 2.8 GHz. The DE parameters using in all cases were $CR= 0.8$ and $F= 0.75$, and 100 individuals pear generations and 20,000 total function evaluations. For BUMDA use 60 individuals per generation with a total 3000 function evaluation and the parameter of truncate population is 1/3. These parameters were obtained through a tuning process.

4.1. Analysis performance of DE and BUMDA stochastic algorithms

Despite, that in last years, the use of the stochastic algorithms to optimization of distillation systems in chemical engineering has been increased, all researchers have been focused in applying algorithms inspired in nature phenomena such as Genetic Algorithm, Simulated Annealing and Differential evolution, obtaining good results but require effort high computation and a long computing time finding one feasible zone. Recently has been design a new generation of algorithms that are based on the estimation of the distribution, called Evolutionary distribution algorithms (EDAs).

For this reason, the aim main of this paper is the performance comparison between DE and BUMDA. The first algorithm is inspired in natural phenomena and the second algorithm is based in estimation of Boltzmann distribution. We compare the computing time, quality solution and avoid getting trapped by local minima. The statistical analysis of the results is realized and determinate which is the better algorithm to optimize distillation systems.

Fig. 6 shows the behavior of the DE and BUMDA algorithms throughout the optimization process for the three case studies analyzed. On the left side are the graphs of the BUMDA and on the right side are those of the DE. For the DE, a similar behavior is observed in the three case studies. Graphs b, d, and f describe a good exploration process and yield good quality solutions that satisfy the constraints imposed by each problem.

On the other hand, the BUMDA describes a very different behavior from that presented by the DE. For all three cases, the BUMDA shows different convergence zones to feasible solutions. In most cases, the feasible zone found improves the objective function value as the number of function evaluations increases. With this behavior it is evident that the BUMDA is capable of departing from local optima. BUMDA during the first generations performs a wide exploration process. When it finds a feasible area, it intensifies the search until the threshold value of the variance is maintained for 5 generations. When this happens and the total number of function evaluations has not been reached, it activates the variance re-initialization mechanism that allows to widen again the search space and eventually, to find a better feasible zone, as shown in graphs a, c and e. This behavior could be observed during the optimization process in the 30 experiments performed, for each algorithm in each case of study.

In this paper, an experiment represents an optimization run that is performed for a given algorithm and a given case study. We decided to perform 30 experiments for each case study, to perform the comparison of the DE and BUMDA algorithms, through statistical tests.

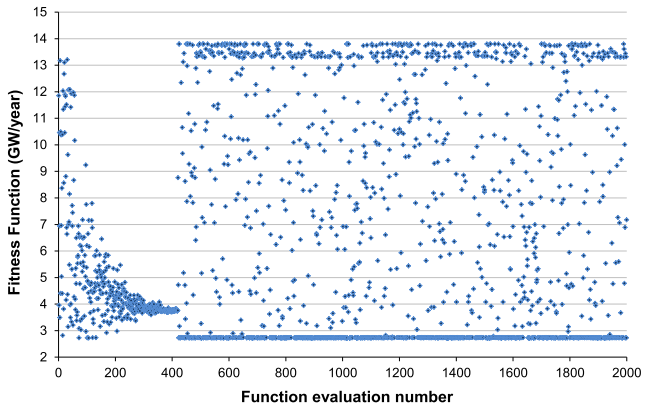
Fig. 7 shows a representative sample of the best solutions found by both algorithms for each case study. The algorithms are compared in terms of the total number of stages and the total energy required in the distillation system in the Fig. 7a, 7c and 7e. The blue points represent the solutions of the DE and the pink points belong to the BUMDA. A blue line and a pink line have been added to represent the average DE and BUMDA, respectively. From this graph, it can be seen that the best solutions found by BUMDA outperform those of the DE due to the fact that most of the designs offer lower values in heat duty and total number of stages. Therefore, the mean value of BUMDA is lower than the mean value of DE solutions. This behavior is observed in the three case studies analyzed.

On the other hand, these graphs show the importance of handling the total number of stages as a constraint within the optimization problem in distillation columns. When the number of stages in a column decreases, the heat duty increases substantially. Therefore it is necessary to have tools that offer designs that decrease both the heat duty and the total number of stages, as shown in Fig. 7a, 7c and 7e.

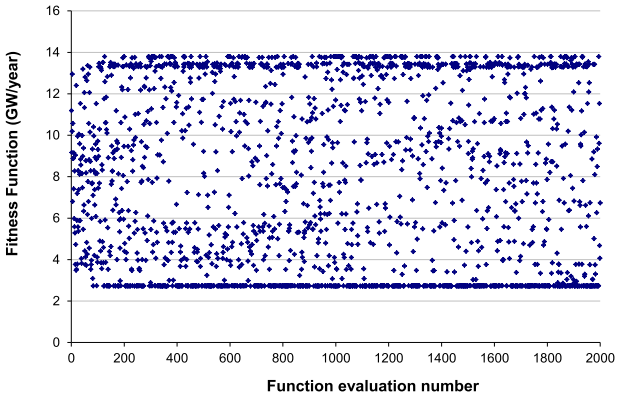
As a complement, Fig. 7b, 7d and 7f shows the box plots for each case study. In this figure, the red line shows the median of each algorithm. This analysis was performed on the 30 solutions corresponding to each experiment. In all three cases, the median of the BUMDA is better than that of the DE. In the case of the quaternary column, Fig. 7f, the DE shows outliers due to the complexity of the distillation system. While the BUMDA shows a bias to the left as its values are more clustered below the median. For the binary column (Fig. 7b), the BUMDA shows a uniform distribution of the data so that the mean, mode and median are very similar, while DE shows a bias to the left. Finally, for the distillation column, DE shows a uniform distribution and BUMDA shows a skew to the right (Fig. 7d).

To make the comparative analysis between the results obtained by the BUMDA and DE algorithms more reliable, the nonparametric statistical test Bootstrap, which is one of the most widely accepted resampling statistical tests, has been implemented. This test has been used to compare the performance of evolutionary algorithms on benchmark functions (Segovia-Domínguez et al., 2020).

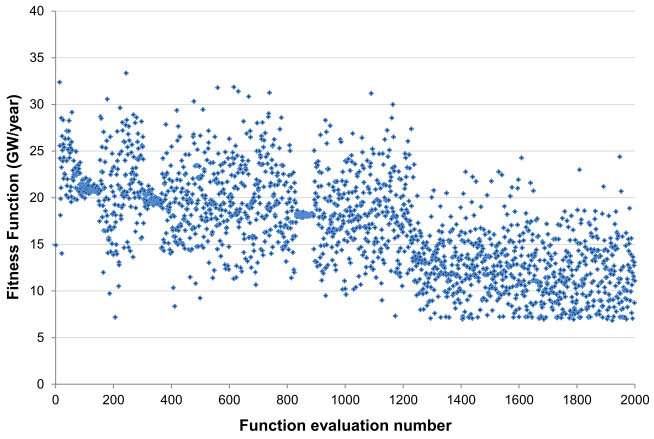
The advantage of Bootstrap is that, being a non-parametric statistical test, it requires assuming theoretical a priori formulations (hypotheses)



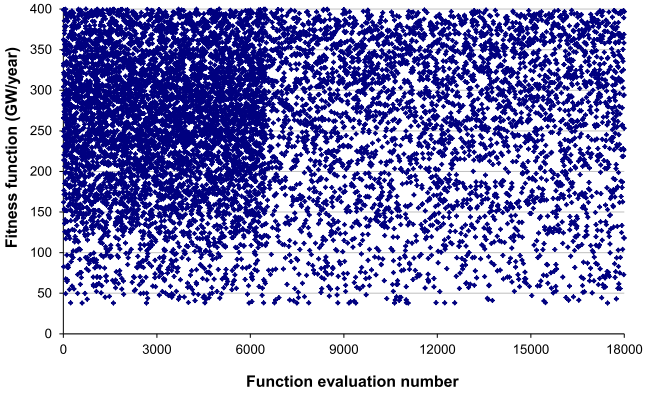
a) Binary column, BUMDA



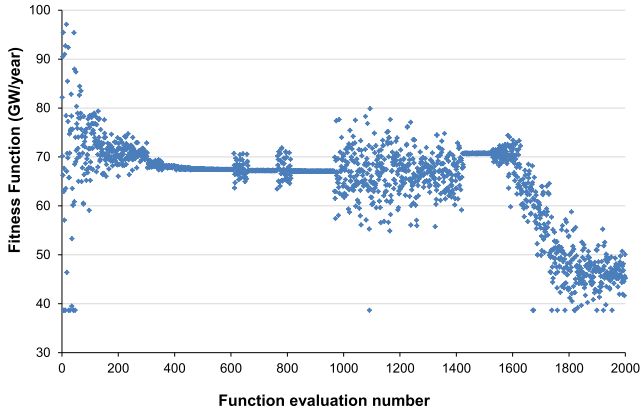
b) Binary column, DE



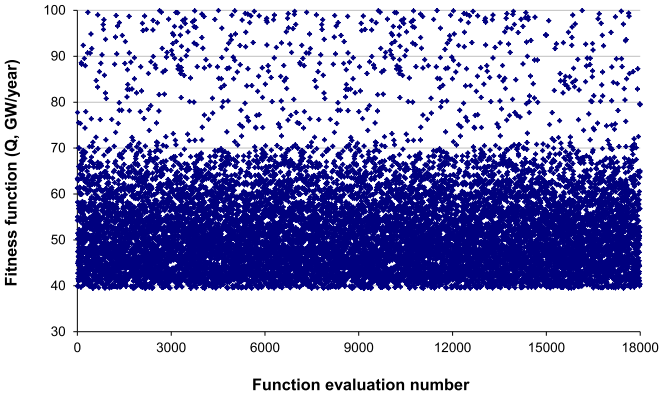
c) Distillation train, BUMDA



d) Distillation train, DE



e) Quaternary column, BUMDA



f) Quaternary column, DE

Fig. 6. Performance of the BUMDA and DE throughout the optimization process.

and can be used for any estimator (mean, median, standard deviation). For the analysis proposed in this study, 3 cases are proposed:

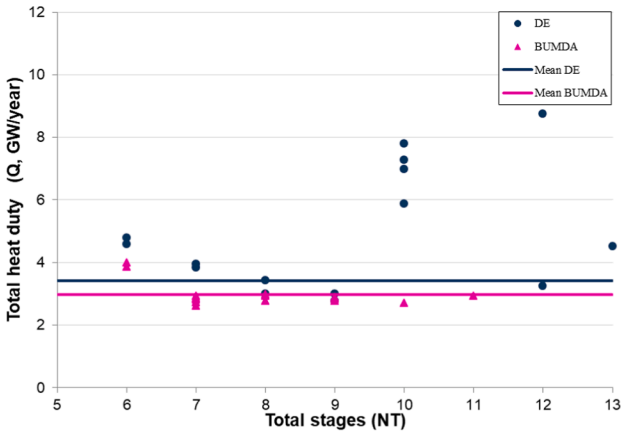
Case 1. The null hypothesis is accepted, defining that the second algorithm performs better.

$H_0 : \mu_1 - \mu_2 \geq 0 H_1 : \mu_1 - \mu_2 < 0$

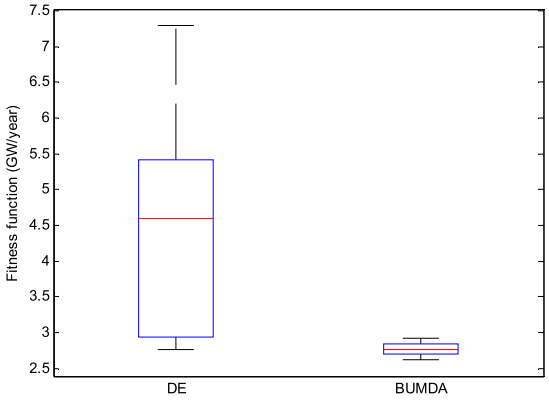
Case 2. The null hypothesis is accepted, there is no substantial evidence of difference in the performance of the algorithms.

$H_0 : \mu_1 - \mu_2 = 0 H_1 : \mu_1 - \mu_2 \neq 0$

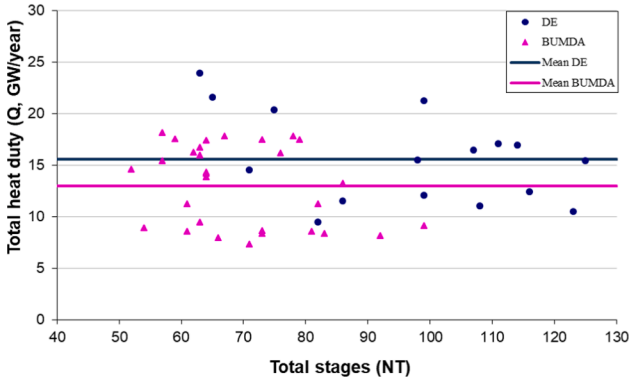
Case 3. The null hypothesis is accepted; the first algorithm has a better performance.



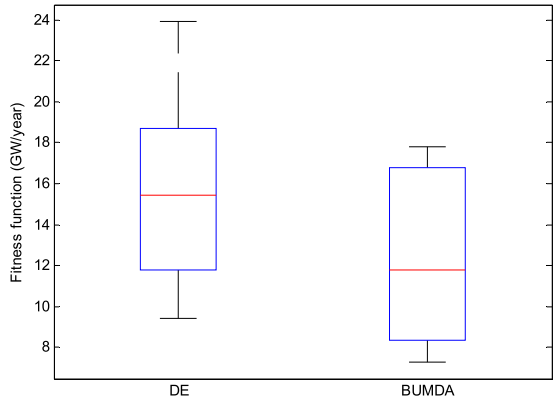
a) Q vs NT, binary column



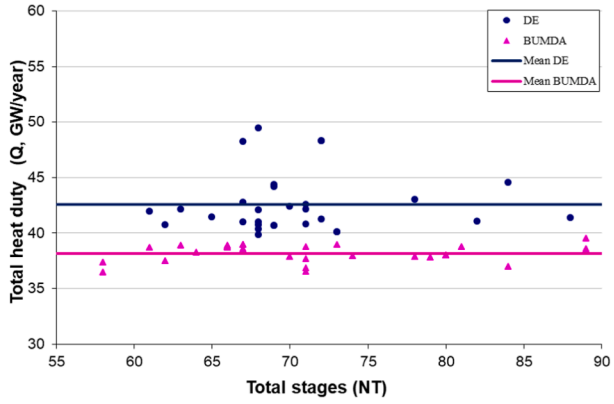
b) DE vs BUMDA, binary column



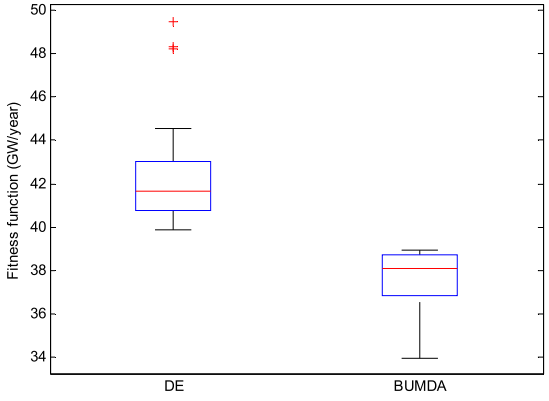
c) Q vs NT, Distillation train



d) DE vs BUMDA, Distillation train



e) Q vs NT, Quaternary column



f) DE vs BUMDA, Quaternary column

Fig. 7. Representative solutions of the experiments performed for the DE and BUMDA algorithms, in each case study.

$H_0 : \mu_2 - \mu_1 \geq 0 H_1 : \mu_2 - \mu_1 < 0$.

This hypothesis was tested using the three cases studied. The 30 solutions found were use as input to Bootstrap tool. The application of the Bootstrap test to determine if there are significant differences in the quality of the set of solutions yielded by each of the algorithms and in turn, if these differences exist, to determine which of the two algorithms has a better performance. In the hypothesis test, μ_1 and μ_2 represent the mean of DE and BUMDA, respectively.

These data were entered into the Bootstrap statistical test to perform the statistical comparison of the results with the mean being the test statistic. The comparison was performed only between ED and BUMDA. For the ED-BUMDA algorithm pair, the statistical tool shows that: there is a significant difference in the solutions found by each algorithm and statistically the best optimal solutions are found by the BUMDA, in all cases. The p-values obtained are 0.9984, 0.9993 and 0.9988 for the first

hypothesis proposed; for binary column, distillation train and quaternary column, respectively. Based on the data analysis for the specific problem shown, it is possible to state with 95 % confidence that the BUMDA performs better, so that it finds better solutions than Differential Evolution.

Table 4 shows several parameters that allow us to compare both the performance of the algorithms and the results obtained in the bootstrap statistical test. The first comparative parameter is the number of function evaluations (NEF). In all cases, DE evaluated 20,000 functions and BUMDA 3000, corresponding to 200 and 50 generations, respectively. This significantly reduces the computational complexity of BUMDA. The solution of the distillation systems varies between 8 and 14 h for the most complex case. For DE, the solution time is between 47 and 112 h.

Respect at the quality solution, we consider two issues:

- Fitness function: Is the total energy consumption in the distillation system. The value obtained by BUMDA is better than DE, in all cases. In the major of the cases study, the worst solution obtained by BUMDA requires the same energy consumption that the best solution of DE.
- Total stages number: It is the sum of the total number of stages of all the columns in the distillation system. In general, BUMDA give design that requires less total stages, so that the size of column is small, in all cases.

On the other hand, to perform the bootstrap test, the level alpha in the 0.05 and in all cases of study when comparing DE with BUMDA, the result shows that BUMDA is better than DE.

Fig. 8 shows radar plots for each case study. The axes correspond to the design variables and the fitness function (total heat duty). These values have been normalized in each dimension with respect to the maximum value found. The blue line corresponds to the best design obtained by DE and the orange line represents the best solution found by BUMDA. In all cases, it is evident that the best solution obtained by BUMDA is better than the best solution obtained by DE. It is also seen that as the distillation system becomes more complex, the BUMDA shows better performance, significantly improving the design obtained by DE, as observed in Fig. 8b).

Finally, based on the results obtained with both algorithms in the three case studies, the stochastic algorithm based in Boltzmann distribution, BUMDA implemented by us, is better than DE, due that offers best solutions in less computing time and requires low effort of computation. Addition the performance in optimization process of BUMDA, presents a high convergence in best feasible zone and is identified clearly an intensification zone that means improve quality of solutions. According results, the BUMDA is capable of explore in all search space and it finds several feasible zones and starts the intensification process in the best feasible zone. This study verifies that the approach presented in this paper, BUMDA with self-adaptive constraints handling technique, is a powerful and robust tool capable of optimizing distillation systems in chemical engineering and potentially useful in other engineering areas.

The numerical results reveal that both DE and BUMDA achieve significant heat duty savings. BUMDA converges faster and reaches a lower heat duty than DE in most cases. However, BUMDA demonstrates better robustness in escaping local optima and finding feasible solutions for more complex problems with stringent constraints.

The convergence plots show that DE improves the solution quality in the first generations, but the progress slows down as it approaches the optimum. In contrast, BUMDA exhibits a more gradual improvement due to being able to avoid local optimum, throughout the optimization process. The final heat duty values for DE and BUMDA shows significant differences, BUMDA outperforming DE in all cases studied. In addition, the BUMDA shows a major performance in complex problems.

5. Conclusions

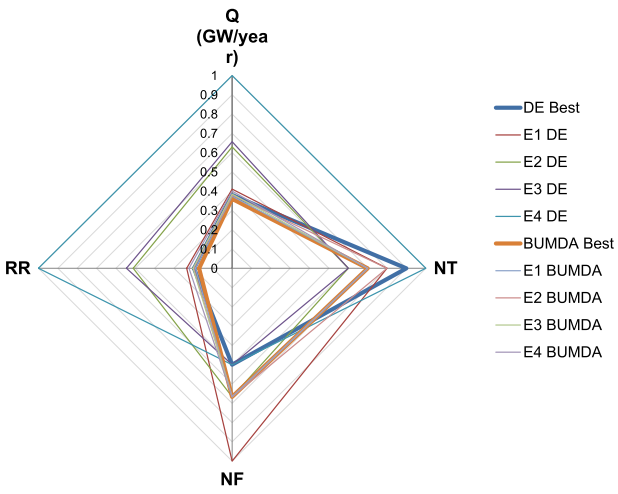
This study demonstrates the effectiveness of the Boltzmann Univariate Marginal Distribution Algorithm (BUMDA), based on the Boltzmann distribution, as a powerful optimization tool for distillation processes with constraints in chemical engineering. When coupled with a self-adaptive constraint handling technique, BUMDA efficiently identifies the optimal solution by aligning the maximum of the Boltzmann distribution with the best fitness function value. The algorithm significantly reduces computational effort, time, and the number of function evaluations required for optimizing complex separation schemes.

The variance re-initialization feature of BUMDA allows for effective exploration of the search space, intensification in promising regions, and the ability to escape local optima. A comparative analysis with Differential Evolution (DE) highlights substantial differences in both the time to obtain a solution and the quality of the results. BUMDA consistently outperforms DE in terms of solution quality across all the distillation systems analyzed, achieving heat duty reductions of 5–20 %, with the highest reductions observed in systems with greater numbers of design variables.

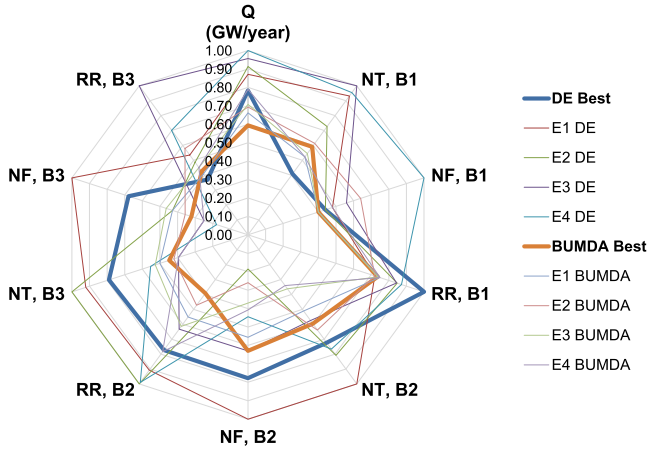
Moreover, the statistical results from the bootstrap test confirm that BUMDA provides the best objective function values in all cases studied. These findings underscore the potential of BUMDA as an effective and efficient optimization tool for distillation system design, particularly when dealing with problems involving a large number of design variables.

Table 4
Performance comparison table between BUMDA and DE algorithms.

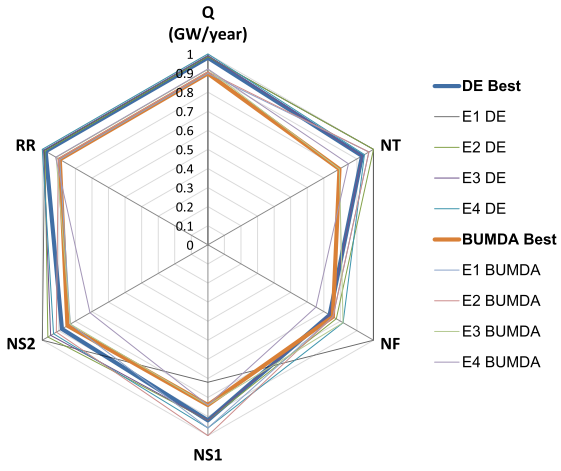
Parameter		Case 1		Case 2		Case 3	
		DE	**BUMDA**	**DE**	**BUMDA**	**DE**	**BUMDA**
Performance algorithms	**NEF**	20,000	3000	20,000	3000	20,000	3000
	Generations	200	50	200	50	200	50
	Operators	F= 0.8, CR= 0.75	Φ= 1/3 Re-init of variance	F= 0.8, CR= 0.75	Φ= 1/3 Re-init of variance	F= 0.8, CR= 0.75	Φ= 1/3 Re-init of variance
	Time solution (h)	47	8	94	12	112	14
	NT	9	7	82	71	68	58
	Q (GW/year)	2.769	2.624	9.426	7.153	39.861	36.498
Bootstrapp testing	**P value**	0.9984		0.9993		0.9988	
	alpha	0.05		0.05		0.05	
	$H_0 : \mu_1 - \mu_2 \geq 0$	**Accepted**		**Accepted**		**Accepted**	
	$H_1 : \mu_1 - \mu_2 < 0$	***(DE equal or worse than BUMDA)***		***(DE equal or worse than BUMDA)***		***(DE equal or worse than BUMDA)***	
	$H_0 : \mu_1 - \mu_2 = 0$	Rejected		Rejected		Rejected	
	$H_1 : \mu_1 - \mu_2 \neq 0$	*(DE and BUMDA are different)*		*(DE and BUMDA are different)*		*(DE and BUMDA are different)*	
	$H_0 : \mu_2 - \mu_1 \geq 0$	Rejected		Rejected		Rejected	
	$H_1 : \mu_2 - \mu_1 < 0$	*(BUMDA better than DE)*		*(BUMDA better than DE)*		*(BUMDA better than DE)*	



a) Binary column



b) Distillation train



c) Quaternary column

Fig. 8. Comparative analysis between the best designs found by DE and BUMDA algorithms, for each case study.

Declaration of Competing Interest

The corresponding author, Juan-Gabriel Segovia-Hernandez is an editor for the journal Chemical Engineering Research and Design, but has had no access to, or involvement in, the peer review process for this paper or its handling by the journal at any point.

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

References

Andrecovich, M.J., Westerberg, A.W., 1985. An MILP formulation for heat-integrated distillation sequence synthesis. AIChE J. 31 (9), 1461–1474. https://doi.org/10.1002/aic.690310908.

Bauer, M.H., Stichlmair, J., 1996. Superstructures for the mixed integer optimization of nonideal and azeotropic distillation processes. Comput. Chem. Eng. 20, S25–S30. https://doi.org/10.1016/0098-1354(96)00015-4.

Cardoso, M.F., Salcedo, R.L., de Azevedo, S.F., Barbosa, D., 2000. Optimization of reactive distillation processes with simulated annealing. Chem. Eng. Sci. 55 (21), 5059–5078. https://doi.org/10.1016/S0009-2509(00)00119-6.

Chen, Q., Grossmann, I.E., 2017. Recent developments and challenges in optimization-based process synthesis. Annu. Rev. Chem. Biomol. Eng. 8 (1), 249–283. https://doi.org/10.1146/annurev-chembioeng-080615-033546.

Cheng, J.K., Lee, H.Y., Huang, H.P., Yu, C.C., 2009. Optimal steady-state design of reactive distillation processes using simulated annealing. J. Taiwan Inst. Chem. Eng. 40 (2), 188–196. https://doi.org/10.1016/j.jtice.2008.10.003.

Cortez-González, J., Hernández-Aguirre, A., Murrieta-Dueñas, R., Gutiérrez-Guerra, R., Hernández, S., Segovia-Hernández, J.G., 2023. Process optimization using a dynamic self-adaptive constraint handling technique coupled to a differential evolution algorithm. Chem. Eng. Res. Des. 189, 98–116. https://doi.org/10.1016/j.cherd.2022.11.006.

Cortez-Gonzalez, J., Segovia-Hernández, J.G., Hernández, S., Gutiérrez-Antonio, C., Briones-Ramírez, A., Rong, B.G., 2012. Optimal design of distillation systems with less than N− 1 columns for a class of four component mixtures. Chem. Eng. Res. Des. 90 (10), 1425–1447. https://doi.org/10.1016/j.cherd.2012.02.004.

Cui, C., Zhang, X., Sun, J., 2019. Design and optimization of energy-efficient liquid-only side-stream distillation configurations using a stochastic algorithm. Chem. Eng. Res. Des. 145, 48–52. https://doi.org/10.1016/j.cherd.2019.03.001.

Errico, M., Rong, B.G., Tola, G., Turunen, I., 2009. A method for systematic synthesis of multicomponent distillation systems with less than N-1 columns. Chem. Eng. Process.: Process.Intensif. 48 (4), 907–920. https://doi.org/10.1016/j.cep.2008.12.005.

Petlyuk, F.B., 1965. Thermodynamically optimal method for separating multicomponent mixtures. Int. Chem. Eng. 5, 555–561.

Fulgueras, A.M., Kim, D.S., Cho, J., 2018. Modeling and optimization study of pressure-swing distillation for the separation process of acetone–methanol mixture with vapor–liquid equilibrium analysis. J. Chem. Eng. Jpn. 49 (2), 84–96. https://doi.org/10.1252/jcej.14we424.

Fulgueras, A.M., Poudel, J., Kim, D.S., Cho, J., 2016. Optimization study of pressure-swing distillation for the separation process of a maximum-boiling azeotropic system of water-ethylenediamine. Korean J. Chem. Eng. 33, 46–56. https://doi.org/10.1007/s11814-015-0100-4.

García-Herreros, P., Gómez, J.M., Gil, I.D., Rodríguez, G., 2011. Optimization of the design and operation of an extractive distillation system for the production of fuel grade ethanol using glycerol as entrainer. Ind. Eng. Chem. Res. 50 (7), 3977–3985. https://doi.org/10.1021/ie101845j.

Gutiérrez-Antonio, C., Ojeda-Gasca, A., Bonilla-Petriciolet, A., Segovia-Hernández, J.G., Briones-Ramírez, A., 2014. Effect of using adjusted parameters, local and global optimums, for phase equilibrium prediction on the synthesis of azeotropic distillation Columns. Ind. Eng. Chem. Res. 53 (4), 1489–1502. https://doi.org/10.1021/ie4019885.

Hanke, M., Li, P., 2000. Simulated annealing for the optimization of batch distillation processes. Comput. Chem. Eng. 24 (1), 1–8. https://doi.org/10.1016/S0098-1354(00)00317-3.

Hu, Z., Li, P., Liu, Y., 2022. Enhancing the performance of evolutionary algorithm by differential evolution for optimizing distillation sequence. Molecules 27 (12), 3802. https://doi.org/10.3390/molecules27123802.

Jia, S., Qian, X., Yuan, X., 2017. Optimal design for dividing wall column using support vector machine and particle swarm optimization. Chem. Eng. Res. Des. 125, 422–432. https://doi.org/10.1016/j.cherd.2017.07.028.

Amminudin, K.A., Smith, R., Thong, D.C., Towler, G.P., 2001. Design and optimization of fully thermally coupled distillation columns: Part 1: preliminary design and optimization methodology. Chem. Eng. Res. Des. 79 (7), 701–715. https://doi.org/10.1205/026387601753192028.

Keßler, T., Kunde, C., McBride, K., Mertens, N., Michaels, D., Sundmacher, K., Kienle, A., 2019. Global optimization of distillation columns using explicit and implicit surrogate models. Chem. Eng. Sci. 197, 235–245. https://doi.org/10.1016/j.ces.2018.12.002.

Kim, J.K., Wankat, P.C., 2004. Quaternary distillation systems with less than N− 1 columns. Ind. Eng. Chem. Res. 43 (14), 3838–3846. https://doi.org/10.1021/ie030640l.

Larrañaga, P., & Lozano, J.A. (Eds.). (2012). Estimation of distribution algorithms: A new tool for evolutionary computation (Vol. 2). Springer Science & Business Media.

Li, J., Du, J., Zhao, Z., Yao, P., 2015. Efficient method for flexibility analysis of large-scale nonconvex heat exchanger networks. Ind. Eng. Chem. Res. 54 (43), 10757–10767. https://doi.org/10.1021/acs.iecr.5b00237.

Lockhart, F.J., 1947. Multi-column distillation of natural gasoline. Petrol. Refin. 26 (8), 14.
Martins, F., Costa, C.A., 2010. Economic, environmental and mixed objective functions in non-linear process optimization using simulated annealing and tabu search. Comput. Chem. Eng. 34 (3), 306–317. https://doi.org/10.1016/j.compchemeng.2009.10.015.
Masoumi, M.E., Kadkhodaie, S., 2012. Optimization of energy consumption in sequential distillation column. World Acad. Sci. Eng. Technol. 6 (1), 67–80.
Modla, G., Lang, P., 2012. Removal and recovery of organic solvents from aqueous waste mixtures by extractive and pressure swing distillation. Ind. Eng. Chem. Res. 51 (35), 11473–11481. ⟨http://pubs.acs.org.ie300331d_si_002⟩.
Modla, G., Lang, P., Denes, F., 2010. Feasibility of separation of ternary mixtures by pressure swing batch distillation. Chem. Eng. Sci. 65 (2), 870–881. https://doi.org/10.1016/S1570-7946(09)70390-6.
Ochoa-Estopier, L.M., Jobson, M., Chen, L., Rodríguez-Forero, C.A., Smith, R., 2015. Optimization of heat-integrated crude oil distillation systems. Part II: Heat exchanger network retrofit model. Ind. Eng. Chem. Res. 54 (18), 5001–5017. ⟨http://pubs.acs.org.ie503804u_si_001⟩.
Peng, F., Cui, G., 2015. Efficient simultaneous synthesis for heat exchanger network with simulated annealing algorithm. Appl. Therm. Eng. 78, 136–149. https://doi.org/10.1016/j.applthermaleng.2014.12.031.
Preechakul, C., Kheawhom, S., 2009. Modified genetic algorithm with sampling techniques for chemical engineering optimization. J. Ind. Eng. Chem. 15 (1), 110–118. https://doi.org/10.1016/j.jiec.2008.09.00.
Segovia-Domínguez, I., Herrera-Guzmán, R., Serrano-Rubio, J.P., Hernández-Aguirre, A., 2020. Geometric probabilistic evolutionary algorithm. Expert Syst. Appl. 144, 113080. https://doi.org/10.1016/j.eswa.2019.113080.
Segovia-Hernández, J.G., Hernandez, S., Petriciolet, A.B., 2015. Reactive distillation: a review of optimal design using deterministic and stochastic techniques. Chem. Eng. Process.: Process.Intensif. 97, 134–143. https://doi.org/10.1016/j.cep.2015.09.004.
Siirola, J.J., Powers, G.J., Rudd, D.F., 1971. Synthesis of system designs: III. Toward a process concept generator. AIChE J. 17 (3), 677–682. https://doi.org/10.1002/aic.690170334.
Srinivas, M., Rangaiah, G.P., 2007. Differential evolution with tabu list for solving nonlinear and mixed-integer nonlinear programming problems. Ind. Eng. Chem. Res. 46 (22), 7126–7135. https://doi.org/10.1021/ie070007q.
Storn, R., Price, K., 1995. Differential evolution-a simple and efficient adaptive scheme for global optimization over continuous spaces. Int. Comput. Sci. Inst. https://doi.org/10.1023/A:1008202821328.
Storn, R., Price, K., 1997. Differential evolution–a simple and efficient heuristic for global optimization over continuous spaces. J. Glob. Optim. 11 (4), 341–359. https://doi.org/10.1023/A:1008202821328.
Sudibyo, S., Murat, M.N., Aziz, N., 2015. Simulated annealing-Particle Swarm Optimization (SA-PSO): Particle distribution study and application in Neural Wiener-based NMPC. In 2015. 10th Asian Control Conference (ASCC). IEEE, pp. 1–6. https://doi.org/10.1109/ASCC.2015.7244567.
Trespalacios, F., Grossmann, I.E., 2014. Review of mixed-integer nonlinear and generalized disjunctive programming methods. Chem. Ing. Tech. 86 (7), 991–1012. https://doi.org/10.1002/cite.201400037.
Udoeyop, S.U., Oboh, I.O., Afiakinye, M.O., 2018. Algorithms for the optimization of well placements—a comparative study. Adv. Chem. Eng. Sci. 8 (2), 101–111. https://doi.org/10.4236/aces.2018.82007.
Valdez, S.I., Hernández, A., Botello, S., 2013. A Boltzmann based estimation of distribution algorithm. Inf. Sci. 236, 126–137. https://doi.org/10.1016/j.ins.2013.02.040.
Valdez, S.I., Hernandez-Aguirre, A., Botello-Rionda, S., 2008. Designing EDAs by using the elitist convergent EDA concept and the Boltzmann distribution. Proceedings of the 10th annual conference on Genetic and evolutionary computation. ACM, pp. 477–478. https://doi.org/10.1145/1389095.13891.
Viswanathan, J., Grossmann, I.E., 1993. An alternate MINLP model for finding the number of trays required for a specified separation objective. Comput. Chem. Eng. 17 (9), 949–955. https://doi.org/10.1016/0098-1354(93)80076-Y.
Wang, L., Pu, Z., Wen, S., 2012. Optimal operation strategies for batch distillation by using a fast adaptive simulated annealing algorithm. Proceedings of the 10th World Congress on Intelligent Control and Automation. IEEE, pp. 2426–2430. https://doi.org/10.1109/WCICA.2012.6358280.
Wang, Y., Bu, G., Wang, Y., Zhao, T., Zhang, Z., Zhu, Z., 2016. Application of a simulated annealing algorithm to design and optimize a pressure-swing distillation process. Comput. Chem. Eng. 95, 97–107. https://doi.org/10.1016/j.compchemeng.2016.09.014.
Weerachaipichasgul, W., Chanpirak, A., Kittisupakorn, P., 2019. Response Surface Methodology in Optimization of Separation Process for Methylal/Methanol Based on Process Simulation of Extractive Distillation. Lecture Notes in Engineering and Computer Science: Proceedings of The International MultiConference of Engineers and Computer Scientists 2019, IMECS 2019, 13-15 March 431–435.
Weinfeld, J.A., Owens, S.A., Eldridge, R.B., 2018. Reactive dividing wall columns: a comprehensive review. Chem. Eng. Process. -Process. Intensif. 123, 20–33. https://doi.org/10.1016/j.cep.2017.10.019.
Xue, F., Liu, L., Chen, X., Shi, X., 2019. Crude oil distillation optimization using surrogate-aided constrained evolutionary optimization. 2019 IEEE Congress on Evolutionary Computation (CEC). IEEE, pp. 1118–1125. https://doi.org/10.1109/CEC.2019.8790122.
Yala, O., Rouzineau, D., Thery-Hetreux, R., Meyer, M., 2017. Design and optimization of heat integrated distillation column “HIDiC”. In: Computer Aided Chemical Engineering, 40. Elsevier, pp. 1783–1788. https://doi.org/10.1016/B978-0-444-63965-3.50299-3.
Yeomans, H., Grossmann, I.E., 2000. Optimal design of complex distillation columns using rigorous tray-by-tray disjunctive programming models. Ind. Eng. Chem. Res. 39 (11), 4326–4335. https://doi.org/10.1021/ie0001974.
Yerramsetty, K.M., Murty, C.V.S., 2008. Synthesis of cost-optimal heat exchanger networks using differential evolution. Comput. Chem. Eng. 32 (8), 1861–1876. https://doi.org/10.1016/j.compchemeng.2007.10.005.
Zhu, Z., Xu, D., Liu, X., Zhang, Z., Wang, Y., 2016. Separation of acetonitrile/methanol/benzene ternary azeotrope via triple column pressure-swing distillation. Sep. Purif. Technol. 169, 66–77. https://doi.org/10.1016/j.seppur.2016.06.009.