12TH INTERNATIONAL SYMPOSIUM ON PROCESS SYSTEMS ENGINEERING AND 25TH EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING

PART A

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Study of Performance of a Novel Stochastic Algorithm based on Boltzmann Distribution (BUMDA) coupled with self-adaptive handling constraints technique to optimize Chemical Engineering process

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Abstract

The optimal design of distillation systems is a highly non-linear, multivariable and multimodal problem. The rigorous model of distillation columns is represented by mass, equilibrium, sum and heat equations called MESH equations and phase equilibrium calculations (Thermodynamic model). Furthermore, it has several local optimums and is subject to several kind constraints such as, design and topology scheme constraints, and achieves targets of purity and recovery for each split component. In this paper, we propose the employment of a novel stochastic algorithm called Boltzmann Univariate Marginal Distribution Algorithm (BUMDA, Valdez, S. I. et al., 2013) coupled with self-adaptive handling constraints technique to optimize a well-known distillation process scheme. The optimization problem consists in minimizing the total reboiler duty in a distillation train to split a mixture made of four components. The BUMDA's performance is compared with Differential Evolution (DE) due to the fact that this last algorithm is used frequently in the optimization of distillation columns. The results show that the BUMDA algorithm is better than the DE algorithm regarding effort computing, quality solution, and time used to find solution. The BUMDA algorithm is efficient, trusted, easy to use and of general applicability in any chemical engineering process.

Keywords: Optimization, BUMDA, Stochastic Algorithms, Distillation train, EDA's.

1. Introduction

The optimization of a distillation system is considered a computer problem of large proportion with a significant number of strongly nonlinear equations that cause serious numerical difficulties when solving the model. Nowadays, this optimization problem is tackled with deterministic and stochastic approaches. Deterministic strategies tackle the problem considering the sequence as superstructures which can be solved with mixed-

integer linear programming and non-linear programming approaches; other authors consider reduced models. On the other hand, the stochastic algorithms can deal with multi-modal and non-convex problems in an effective way and without the mentioned limitations. They are a suitable alternative to the design and optimization of complex separation schemes. In chemical engineering processes, distillation is a widely used separation process and a very large consumer of energy. A great amount of research has been carried out to improve the energy efficiency of distillation systems, in terms of either the design of optimal distillation schemes or improving internal column efficiency. Nowadays, the optimal design of multicomponent distillation systems remains one of the most challenging problems in processes engineering.

In this work, BUMDA algorithm performance is compared with Differential Evolution algorithm (DE) due to the fact that it is one of the most used evolutionary algorithms for solving global optimization problems in chemical engineering processes (R. Vakili et. al., 2011; Cabrera-Ruiz et. al., 2011). Both algorithms were coupled with self-adaptive handling constraints technique and were employed to optimize a distillation train that split a four components mixture.

2. Case study

In chemical engineering processes MESH equations and thermodynamic equilibrium equations have high levels of nonlinearities and nonconvexities and also present convergence difficulties. This leads to high computational times and the requirement of good initial guesses and bounds on the variables to achieve convergence.

Following case of study is described. The objective of a distillation train is to separate a multicomponent mixture using only single columns. Each column receives a feed-in and carries out the distillation of two adjacent components (adjacent volatility), and delivers two products: one at the top and the other at the bottom. In order to separate a mixture of *N* components, it is necessary to use *N-1* single columns. The order in which the components are separated is based on their relative volatility (Figure 1).

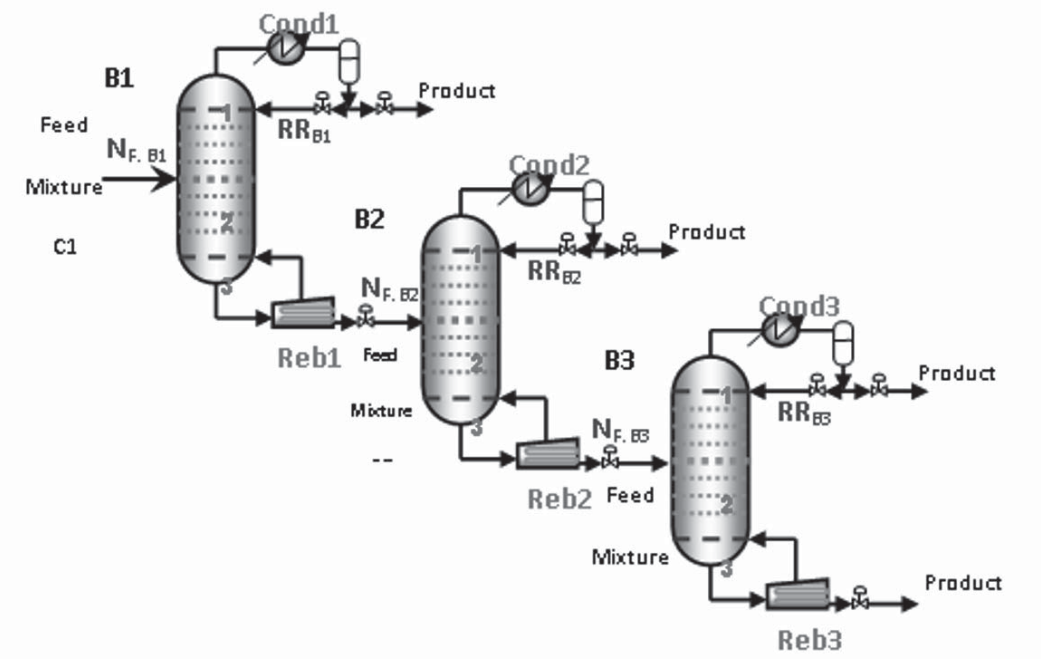

Figure 1. Flowsheet of distillation train to split a mixture of four components.

The basic design of each distillation column requires finding the best values of: the total number of stages *NT*, feed stage *NF* and reflux ratio *RR*, which is the relationship between the liquid flow *L* that returns to the column and the vapor flow *V* that rises in the column.This takes places on the upper part of the column. With this set of variables, the main goal of design is to obtain the minimum total heat duty possible to achieve the separation of the mixture. In mathematical terms, the problem statement optimization is described as following:

Find vector

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

To minimize fitness function

$$Q = f(Z)$$

Subject to constraint function

$$g_{1,j}(Z) = x^{\text{pur}}_{\text{target}} \qquad j = 1,...,M_{\text{constraints}}$$

$$g_{2,j}(Z) = x^{\text{rec}}_{\text{target}} \qquad j = 1,...,M_{\text{constraints}}$$

And subject to boundary constraints

$$z_i^{(L)} \le z_i \le z_i^U \qquad i = 1,...,D$$

$$2 < NF_{Bl} \le NT_{Bl} \qquad l = 1,...,B_{columns}$$

Where for each column *B*, *NT* is the total number of stages and *NF* is the number of feed stage. These dimensions are discrete variables and *RR* is the reflux ratio. These are continuous variables; in total we have nine dimensions, of which six are discrete and three are continuous. The fitness function is to minimize the total heat reboiler duty *Q* that is a function of vector *Z*. Regarding the design constraint, we have two types: one is referred to as purity, and other one as recovery; these exist for each component. Also it is important to consider the boundary constraints, because *NF* should always be less than *NT* and each dimension, *Zi* is between lower and upper boundaries.

3. Optimization strategy

In this research, we chose two stochastic algorithms: Differential Evolution (Viswanathan, J. and Grossmann, I. E., 1993). Which generates new points that are perturbations of existing points, and Boltzmann Univariate Marginal Distribution Algorithm BUMDA (Valdez, S. I. et al., 2013), that uses a normal distribution to approximate the Boltzmann Distribution, using the mean and variance of the population. These algorithms are coupled with self-adaptive handling constraints that allow use to find feasible solutions that achieve all design and specification constraints throughout distillation column optimization. Furthermore, it is important to mention that the optimization approach has been developed using an interface which links the optimizer algorithms with the modular simulator through databases. Following the characteristics of the algorithms, technique of handling constraints and optimization approach are briefly described.

3.1. Boltzmann Univariate Distribution Algorithm (BUMDA)

EDA's use a probability distribution, called the search distribution, to sample new candidate solutions. Hence, the search strategy in EDA's is to increment the probability of sampling the optimum from the search distribution. The advantage of the BUMDA algorithm is the preservation of the desired characteristics of the Boltzmann distribution,

while maintaining a low computational cost in the estimation and sampling steps. It also focuses on sampling as many promising solutions as possible, avoiding sampling promising and non-promising solutions and then rejecting some of them. The BUMDA algorithm starting with a population is initialized between the bounds of the search space and the fitness function calculated. 30% of the best individuals are stored in the selected set, and used to compute the mean and variance parameters of the Normal distribution. Then new individuals are simulated from a Normal distribution with such parameters to populate the next generation.

3.2. Differential Evolution (DE)

Differential evolution is proposed by Storn and Price (Storn, R. and Price, K., 1995). DE is a stochastic direct search method using population or multiple search points. DE has been successfully applied to the optimization problems including non-linear, non-differentiable, non-convex and multi-modal functions. It has been shown that DE is fast and robust when applied to these functions. In DE, initial individuals are randomly generated within the search space and form an initial population. Each individual *i* contains *D* genes as decision variables or a decision vector *Zi*. At each generation or iteration *G*, all individuals *Npob* are selected as parents. Each parent is processed as follows: the mutation process begins by choosing three individuals from the parents except for the parent in the processing. The first individual is a base vector. Subsequent individuals are paired to create difference vectors. The difference vectors are scaled by the scaling factor *F* and added to the base vector. The resulting vector is then mated or recombined with the parent. The probability of recombination at an element is controlled by the crossover factor *CR*. This crossover process produces a trial vector. Finally, for survivor selection, the trial vector is accepted for the next generation if the trial vector is better than the parent.

3.3. Optimization Process

For the optimization approach implemented in this work, we have developed an interface which links the optimizer BUMDA or DE (Master, coded in MatLab) with the modular simulator Aspen Plus (Fitness Function Evaluator) through the Excel (Database). In this interface the stochastic algorithm needs one individual physically feasible of beginning the optimization process. Here, physically feasible implies that for a distillation column, the feed stage must be smaller than the total number of stages, and the reflux ratio is greater than zero. The stochastic algorithm generates individuals with the proper dimensionality, which is sent to Aspen Plus, one by one, in order to simulate the distillation scheme and get the values of the fitness function evaluated with constraints.

4. Discussion and Results

In this paper, a comparative analysis of performance ED and BUMDA stochastic algorithms is presented. Many authors have used ED algorithm to optimize chemical engineering problems while the BUMDA algorithm has been used only once. Both algorithms are tested to optimize two well-known problems in chemical engineering. The problem is to purify a four aliphatic hydrocarbons mixture in a distillation train. We carried out tuning of parameters in two algorithms. The total number of evaluation is the stop criterion and the fitness function is the total heat duty minimization. The simulations were carried out with a PC computer with an i5 processor core, clock frequency at 2.8 GHz, and 8 GB of RAM. In this case we study a mixture made of four lineal aliphatic hydrocarbons fed at a flow-rate of 100 kmol/h; which is introduced in the first column as saturated liquid. The characteristics and constraints of the mixture

are presented in Table 1. The proportion of each component is shown in mol fraction. Each component must be delivered with the specified purity and recovery. The design pressure for the separation was chosen to ensure that cooling water was used in the condensers. The phase equilibrium for liquid of this mixture is calculated with the Chao-Seader model, because it is usually recommended for hydrocarbon mixtures operating at low or medium pressure.

Table 1. Characteristics of the case study.

Characteristics of the mixture			Constraints	
ID	Component	Feed, mol fraction	Purity, x_i^{pur}	Recovery, x_i^{rec}
A	n- butane	0.05	0.987	0.98
B	n- pentane	0.45	0.98	0.98
C	n-hexane	0.45	0.98	0.98
D	n-heptane	0.05	0.986	0.98

4.1. Analysis performance of DE and BUMDA stochastic algorithms

The main aim of this paper is analyze the performance of two algorithms, DE inspired in natural phenomena and BUMDA based in estimation of Boltzmann distribution. The comparative parameters are effort of computation, time that found solution, quality of solution and behavior along optimization process. In Table 2 we analyze three comparative parameters. The first comparison is effort of computation; i.e. maximum number of function evaluations that each algorithm requires to find the best solution. It is clear that the BUMDA algorithm only needs *15 %* of *NEFmax* of what the DE algorithm requires. The time find a solution, is in direct relation with *NEFmax*, so that the BUMDA is faster than the DE algorithm. The BUMDA only requires 8% of the time that DE algorithm requires.

Table 2. Comparative analysis of best individuals obtained by DE and BUMDA algorithms

Parameter	DE Algorithm	BUMDA Algorithm
Effort of computation $\left(NEF^{\max}\right)$	20,000	3,000
Time of solution $\left(\theta, hours\right)$	100	8
Quality solution $\left(Q, BTU/h\right)$	9425750.75	7153129.14
Quality solution $\left(NT^{total}\right)$	84	71

In Figure 2 there are two sets of point: blue points that represent the best solutions given by the DE algorithm and pink points that are the feasible solutions obtained with the BUMDA algorithm. In this graph, the total number of stages is the axis "x" versus total heat duty shown in the "y" axis. Both variables are the most important in the design of distillation columns, since they show the compromise between size column and its energy consumption. It's clear that the pink points are better than blue points, both in *NT* as *Q*. If we compare the best solution only in terms of energy, the best pink point requires around 2,300,000 BTU/h less of the energy consumption than the best blue point; this behavior is similar in total number of stages. Based on these results, the best

solution obtained by the BUMDA algorithm provides the better compromise to design the distillation train.

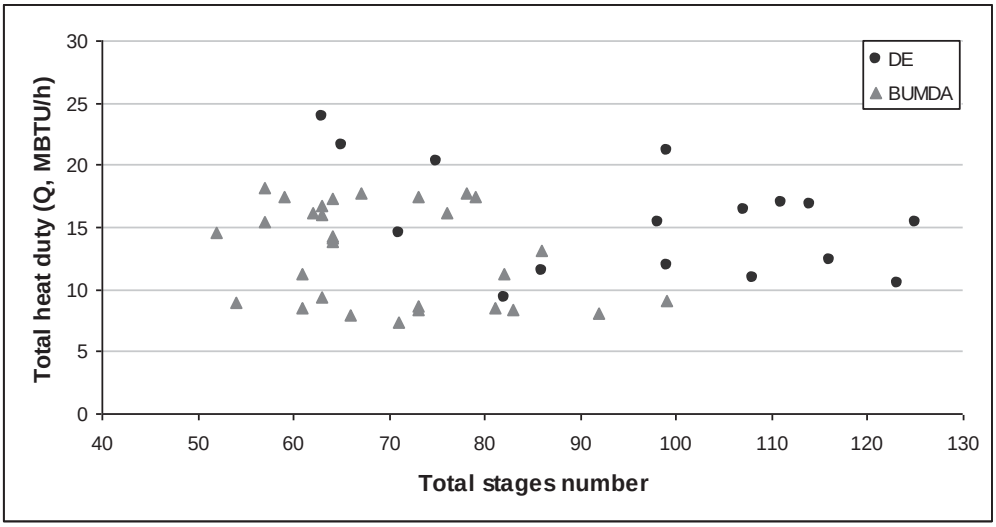

Figure 2. Comparative of the best individuals obtained by DE and BUMDA algorithms.

Finally, based on the results obtained with both algorithms in this case study, the novel stochastic algorithm based on Boltzmann distribution, the BUMDA algorithm implemented by us, is better than the DE algorithm, due to the fact that offers better solutions in less time and requires low computation effort. In addition the performance in optimization process of the BUMDA algorithm presents a high convergence in the best feasible zone and is identified clearly in an intensification zone, which leads to an improvement in the quality of solutions. This study verifies that the approach presented in this paper, BUMDA algorithm with self-adaptive handling constraints technique, is a powerful and robust tool capable of optimizing processes in chemical engineering and is potentially useful in other areas of engineering.

5. Conclusions

In this paper, a comparative study of the general performance of stochastic algorithms to optimize a distillation train is presented. We used two stochastic algorithms: Differential Evolution (ED) and Boltzmann Univariate Marginal Distribution Algorithm (BUMDA). The best solution was found by the BUMDA algorithm. The BUMDA algorithm is better than the DE algorithm because BUMDA is capable of finding the best design with little numeric effort, short computing time and a good success rate.

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