FEED PROFILE OPTIMIZATION OF A BATCH FED ALCOHOLIC FERMENTATION BY USING GENETIC ALGORITHM TO MAXIMIZE ETHANOL PRODUCTION

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Abstract. *This paper aims to develop a mathematical modeling and computer simulations of an alcoholic fermentation with inconstant batch feed. Fermentation is a process with large application in the industry, which objective is to obtain valuable products such as ethyl alcohol, also known as ethanol. Ethyl alcohol production in Brazil is growing fast due to politic investments to reduce pollution levels caused by combustion gases. Produced mainly by the black treacle (molasses), the Brazilian ethanol fermentation may seem simple. However, it is a microbiological process, which means there are many variables to be analyzed as well as the metabolic biochemical reactions and various types of transport phenomena. Economically speaking, evaluate the variables that compose this process becomes an important step in optimizing the production and reducing costs. One of the most important aspects in a batch feed fermentation is the substrate feed profile on the bioreactor, which determines how much ethanol is produced. In this work, a strategy to optimize the parameters of each substrate feeding profile is developed by using objective functions. The goal is to maximize the ethyl alcohol concentration in the product. The Genetic Algorithm (GA) approach is a heuristic method based on the natural selection principle postulated by Darwin as well as the genetic succession principle postulated by Mendel. The GA method has been highlighted in the literature due to its good performance. Thus, in most optimization cases, a GA follows the steps: ability, selection, crossing, mutation, acceptation, exchange, and test. The algorithm was implemented in MATLAB interacting with the objective function to adjust the feed profile parameters, aiming to the maximum ethanol production.*

Keywords: *Optimization, Genetic Algorithm, Fed-Batch Fermentation.*

1 INTRODUCTION

Ethanol fermentation of a large number of agro-industrial residues has been studied in its various forms: batch or continuous (Hjersted & Henson, 2006; Converti et. al., 2003). Laluce (1991) discuss that sugar cane blackstrap molasses can be classified as the most suitable waste materials used for fuel ethanol production, mainly because of its cheap price and abundant quantity in the sugar industry. Looking back to the oil crisis of 1973, Laluce (1991), also reports the importance of the National Alcohol Program (PNA) in the Brazilian economy. The purpose of the program was a reduction of the dependence on imported petroleum for gasoline.

In this scenario, the understanding and evaluation of parameters involved in the ethanol production process is of importance for the country and represents a promissory work field for engineering. The Brazilian ethanol is produced by the alcoholic fermentation of molasses, a process that has complexities inherent to its nature. Fermentation is a microbiological process that involves a large number of variables with a high degree of complexity and dynamic behavior, which brings some difficulties to its operation (ROCHA et al., 2004).

One important factor to be considered in an alcoholic fermentation conducted in fed-batch is the filling profile of the wort. Some authors report the importance of this profile in the literature. Santos et al. (2005) investigated experimentally the yields of ethanol production related to a variety of predefined profiles of feed rates. His work presents a validation of kinetic models from experimental data and different optimization techniques. Levišauskas e Tekorius (2005), on the other hand, suggested the use of mathematical functions with adjustable parameters, which can govern the typical wort feed behavior of the dorna.

Another approach can be found in the work of Coelho et al. (2008) that used the Levenberg-Maquardt mathematical method to optimize parameters of the equations proposed by Levišauskas e Tekorius (2005). The authors report some difficulties during the use of this method, such as, the initial estimative of the parameters, which is made by trial and error.

Aiming to contribute to the investigation of the filling profile in fed-batch fermentation process, this paper investigates the achievement of the maximum ethanol production by adopting a simulation/optimization strategy, which makes use of a Genetic Algorithm (GA) interacting with an objective function to optimize the adjustable parameters for the mathematical functions that represent the predefined parameters of feed.

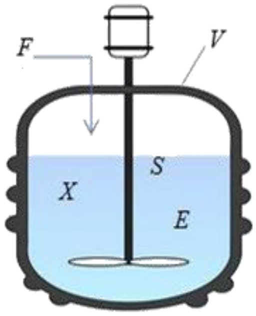
2 METODOLOGY

This paper was developed in two steps: the modelling and simulation of the fermentation process using the kinetic models validated by Torres et al. (2008) and the optimization of the mathematical function parameters responsible for defining the feed profiles using Genetic Algorithm (GA).

1.1.1 Modelling and Simulation

The mathematical model adopted in this work was based on simplifications proposed by Vasconcelos (1987). Figure 1 shows the diferential equations obtained from the mass balance on the batch reactor, as well as the simplification of the equipamente and variables of the process.

Where *X, S, E* and *V* are the concentration of cells, substract, ethanol (g/L) and the reactor volume, respectively. $D = F/V$ represents the dilution effect due to the increase of the volume, being *F* the feed profile, which can be predefined and optimized on the second phase of this work. S_a is the wort concentration that feed the reactor (g/L), $Y_{x/s}$ is the substract-cell yield factor and $Y_{p/s}$ is the substract-ethanol yield factor. μ and γ are the specific growth rate for the cells and ethanol production, respectively, which are parameters intrisec to the kinectic model.



$$\frac{dV}{dt} = F \tag{1}$$

$$\frac{dX}{dt} = (\mu - D) \cdot X \tag{2}$$

$$\frac{dS}{dt} = D \cdot (S_a - S) - X \cdot (\frac{\mu}{Y_{x/s}} - \frac{\gamma}{Y_{p/s}}) \tag{3}$$

$$\frac{dX}{dt} = \gamma \cdot X - E \cdot D \tag{4}$$

Figure 1. Mass balance equations and process variables.

In this context, the choice of some kinectic models are important. Torres et al. (2008) and Coelho et al. (2008), used experimental data of a fermentation with no cell recycle conducted in pilot scale (23 tests) and with recycle in industrial scale (22 tests) to determine the parameters of 8 models. The results show that the Tessier model (BLANCO et al., 2005) has the best fit for industrial scale. For this paper, the Tessier model was adopted to model and simulate the fermentation process using the μ and γ parameters validated Torres et al. (2008).

1.1.2 Genetic Algorithm optimization

Levišauskas e Tekorius (2005) report 4 types of feed profile for the wort. Equations from 5 to 8 show the mathematical functions and the parameters to be optimized.

$$\mathrm{F(t)} = a \tag{5}$$

$$\mathrm{F(t)} = a + bt \tag{6}$$

$$\mathrm{F(t)} = a \cdot \exp(b + ct) \tag{7}$$

$$\mathrm{F(t)} = \sum_{i=1}^{5} \mathrm{w_i} \cdot \exp\left(\frac{-(t - d_i)^2}{\rho_i^2}\right) \tag{8}$$

Parameters *a, b, c,* w_i, d_i, ρ_i must be optimized, and *t* is the filling time wich is not neccessarely the same as fermentation time.

1.1.3 Objective function

For this work the strategy involves the optimization of the parameters show in Equations 5 to 8 by using an objective function. Following the recommendations of Coelho et al. (2008) this paper used Equation 9 as an objective function to maximize the ethanol production.

$$\mathrm{J} = \mathrm{E(t)} \cdot \mathrm{V(t)} \tag{9}$$

Where *E(t)* representes the ethanol concentration and *V(t)*, the volume.

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1.1.4 Genetic Algorithm

Genetic Algorithm was used as the optimization method implemented in Matlab® by using the *ga* function present on the Global Optimization Toolbox. It interacts with the objective function (Equation 9) adjusting the parameters shown in Equations 5 to 8. The linear restrictions applied to the algorithm are treated to guarantee that the results stay in the problem domain limits. GA uses Augmented Lagrangian Genetic Algorithm (ALGA) by combining the fitness function and nonlinear constraints using the Lagrangian and the penalty parameters.

GA is a heuristic optimization method developed by Holland (1975) and based on Darwin's evolution theory and the Mendelian genetic inheritance theory, which indicate a higher survival trend of the more fit individuals and the transfer of genetic information by crossing individuals (SCHWAAB, 2005). GA uses combinations starting from random initial parameters, which Interact with the objective function by following an algorithm that uses the ability, selection, crossing, mutation, acceptation, switch and test steps. At the end, the GA returns the optimized parameters. This method is traditionally operated ignoring the meaning of the manipulated structures, as well as, the way to work over them. Therefore, there is no need of a specific knowledge of the problem domain, which gives GA a generic and robust structure.

3 RESULTS

A quantification of the results is made by evaluatig the GA optimized parameters in each fed profile, as well as, the concentration and volume at the end. The results are shown in Tables 1 and 2.

Table 1. Optimized parameters from the Equations 5 to 8.

Parameters	Equations			Equation 8			
	5	6	7	i	w_i	d_i	ρ_i
a	23,333	46,6680	6,1659	1	1,6468	-2,3852	-1,0638
b	-	-7,7782	2,6526	2	12,5975	0,5537	-1,7981
c	-	-	-0,6088	3	10,8272	-4,4902	6,9003
				4	13,0894	0,7052	-1,2629
				5	13,7896	0,3952	-1,8992

Table 2. Final ethanol concentration and dorna total volume.

Profile	Ethanol concentration (g/L)	Total volume (L)	Profile	Ethanol concentration (g/L)	Total volume (L)
5	37,1162	187,8609	7	43,2729	188,0837
6	37,4692	187,9600	8	39,2783	148,0091

From the results shown in Table 2, the profile 7 achieved the highere ethanol production. GA optimization is satisfatory since the algorithm returned a good response to the evaluated problem with no need for excessive computational effort. Despite GA generic and robust structure, restrictions where implemented as a way to prevent the algorithm to look for solutions outside of the problem domain. These restrictions guarantee that the solution has physical meaning.

CONCLUSIONS

GA utilization to search for solutions on optimization problems as the one shown in this paper is seen as a promissory innovation. A maximum ethanol production was found using the exponential profile. GA's ability to not need an initial estimative allows a more simple solution for the parameters optimization, since the literature does not give data to estimate those parameters. Therefore, the use of the classic optimization with Levenberg-Maquardt would need more time because the initial guess is made by trial and error. Furthermore, GA has returned good responses in a smaller computational time than others heuristic methods in this application, as particle swarm optimization (PSO). It shows the applicability of GA to solve optimization problems similar to the one presented in this paper.

REFERENCES

Blanco, M. ; Peinado, A. C. ; Mas, J. Monitoring Alcoholic Fermentation by Joint use of Soft and Hard Modelling Methods, *Analytica Chimica Acta 556 (2005) 364–373*.

Coelho, F. A., Torres, W. L. S., Carvalho, F. O., Vasconcelos, J. N. Modelagem do processo de fermentação em batelada alimentada e determinação do perfil ótimo de alimentação de mosto. *VIII Congresso Brasileiro de Engenharia Química em Iniciação Ciêntifica.* Minas Gerais BR, Uberlândia, 2009.

Holland, J.H., 1984. Genetic algorithms and adaptation. In: Adaptive Control of Ill-Defined Systems. Springer US, Boston, MA

Levisauskas, D., Tekorius, T. Model-based optimization of fed-batch fermentation processes using predetermined type feed-rate time profiles. A comparative study. *A Comparative Study,* ISSN 1392 -124X Information Technology And Control, 2005, Vol.34, No.3.

Mathworks. Nonlinear Constraint Solver Algorithms. 2017. Available in: < https://www.mathworks.com/help/gads/description-of-the-nonlinear-constraint-solver_bqf8bdd.html> Access in: 30 aug. 2017.

Rocha, M., Neves J., Rocha I., Ferreira, E. C. Evolutionary Algorithms for Optimal Control in Fed-batch Fermentation Processes. *EvoWorkshop 2004, LNCS 3005,* pp. 84-93, 2004.

Santos, K. G., Lobato, F. S., Murata, V. V., *VI Congresso de Engenharia Química em Iniciação Cientifica, UNICAMP 2005.*

Schwaab, M. *Avaliação de Algoritmos Heurísticos de Otimização em Problemas de Estimação de Parâmetros.* Dissertação de Mestrado. Universidade Federal do Rio de Janeiro. Rio de Janeiro. 2005.

Torres, W. S., Carvalho, F. O., Vasconcelos, J. N. Modelagem e simulação da fermentação alcoólica conduzida em batelada alimentada com vazão variável de alimentação. *VII Congresso Brasileiro de Engenharia Química.* Pernambuco BR, Recife, 2008

Vasconcelos. J. N. de. *Operação e Simulação do Processo de Fermentação Alcoólica em Batelada Alimentada com Vazão Variação de Alimentação*. Rio de Janeiro, 1987, 229p.(Dissertação de Mestrado-Escola de Química da UFRJ).