Book of Abstracts
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Dynamic modeling of the acrylic acid synthesis from renewable resources

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1. Summary

The purpose of this work is the model development for the biotechnological process of acrylic acid synthesis. The kinetic model is based on the concepts of structured representation, and adapted from a structured growth model developed by Lei et al. (2001) and a structured model for ethanol production developed by Stremel (2001). The full detailed model is a set of partial differential equations composed by the reactor equations together with the description of the microorganism metabolism aiming to follow the evolution of intracellular variable that are difficult to measure. The reactor is continuously operated and the challenge is to define operating strategy and conditions to achieve the product within the desired specifications. In this work it is used the multivariate analysis techniques, as experimental design to identify the parameters with the most significant impact on the model, to represent well the process as well as to identify a suitable way to adjust the model for the acrylic acid production process. The mapping of the dynamics of the developed process is made using techniques of factorial design together with the methodology of Plackett-Burmann. It is shown that it is possible to increase the process performance by choosing optimized conditions for the reactor operation. After identified the main kinetic and operational parameters of the process, was implemented an optimization strategy for search the optimal operational variables through of the algorithms optimization SQP (Sucessive Quadratic Programming).

Keywords: structured model, acrylic acid, biotechnological process, experimental design, optimization

2. Extended Abstract

A great challenge related to preservation of the environment is the exhaustion of raw material based on oil. With the synthesis of chemical products through biotechnological processes is possible to discovery and to explore innumerable routes that can be used to obtain products of high added value. These routes form parallel and alternative ways for the production of the desired product, what makes easier the environment preservation and a rational use of renewable feedstock. The acrylic acid is one of the most important industrial chemical products. Usually it is obtained by oxidation of propylene. A possible alternative way is the fermentation from sugar cane. A detailed description on the sugar cane can be found in the following references: Calle et al. (2005), NIPE (2007), UNICA (2007). The purpose of this work is the model development for the biotechnological process of acrylic acid synthesis. A continuous bioreactor with immobilized cell of *Saccharomyces cerevisiae* was used in the work. The bioreactor behaviour is based on mass balances for the key chemical species of the fermentative process. The set of partial differential equations is solved coupling the Orthogonal Collocation Method to discretize the radial ordinates with the Method of Lines to integrate the system of equations by a stiff integrator. The main intention of this work is the development of a tool able to represent the main phenomena-taking place in the cell mechanism so that several routes can be explored to achieve a desired product. Figure 1 shows the concentration profiles of acrylic acid and substrate (glucose) obtained in dynamic behaviour of the continuous bioreactor used in process simulation of acrylic acid production. Figure 2 shows the concentration profiles of acrylic acid, biomass and glucose obtained when the steady state is reached.

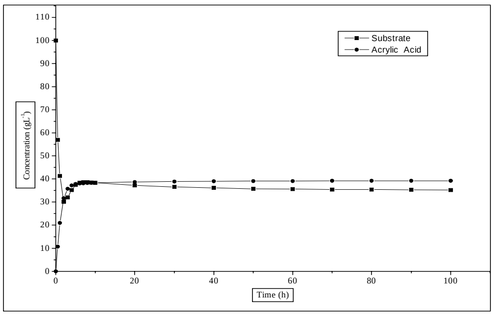

Figure 1: Acrylic acid and substrate concentration

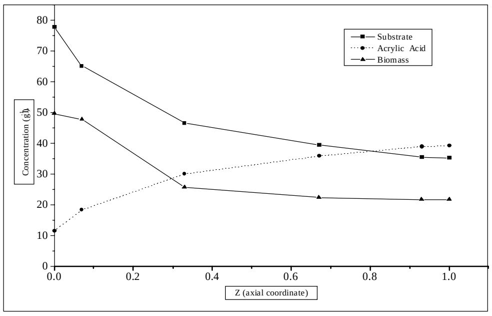

Figure 2 - Acrylic acid, biomass and substrate concentration at long reactor length

In this study, the Plackett-Burmann design and fractional factorial design had been used to identify more significant kinetics and operational parameters of the process of acrylic acid synthesis. The obtained results are shown in Pareto chart (Figure 3 and 4). After identified the main kinetic and operational parameters of the process, was implemented an optimization strategy for search the optimal operational variables through of the algorithms optimization SQP (Sucessive Quadratic Programming).

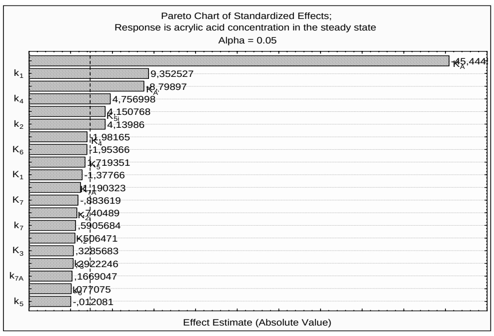

Figure 3: Pareto chart of the kinetic parameters effects

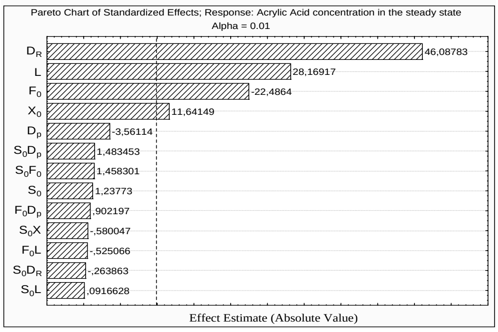

Figure 4: Pareto chart of the operational parameters effects

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