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Dynamics of a continuous flash fermentation for butanol production

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The ABE (acetone, butanol, ethanol) fermentation is characterized by its low productivity. In this paper, this issue is overcome with an innovative industrial process that employs the flash fermentation technology. The process consists of three interconnected units, as follows: fermentor, cell retention system (tangential microfiltration) and vacuum flash vessel (responsible for the continuous recovery of butanol from the broth). The dynamic behaviour of the process is described by a non-linear mathematical model with kinetic parameters determined experimentally. From simulations of the mathematical model the dynamic characteristics of the process were investigated. Analyzes of the open-loop dynamic behavior of the process, after step perturbations in the manipulated variables, determined the best control structures for the process.

1. Introduction

The increasing appeal to search for alternative routes for chemicals production apart from petrochemical route claims for research of green technologies allied to bioprocesses development. This work focuses on an industrial-scale fermentation for biobutanol production. Carrying out the butanol fermentation under optimized operating conditions is essential to run a biobutanol industry that can compete effectively with the current butanol derived from the petrochemical route, since the ABE (acetone, butanol, ethanol) fermentation, as normally is called the fermentation to produce butanol, is characterized by its low productivity. Product toxicity results in low butanol concentration in the reactor. In addition, the use of dilute sugar solution results in large process volumes. Mainly because of these problems and due to high costs related to the distillation of dilute product streams, the production of biobutanol on a commercial scale has been considered to be uneconomical (Ezeji et al., 2007).

During the past two decades a significant amount of research has been performed on the development of alternative technologies designed to remove the butanol continuously

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from the fermentation broth (e.g. adsorption, gas stripping, ionic liquids, liquid–liquid extraction, pervaporation, aqueous two-phase separation, supercritical extraction, perstraction, etc.) (Ezeji et al., 2007). These recovery techniques reduce the effect of product inhibition allowing an increase in the substrate concentration, which results in a reduction in the process streams, higher productivity and lower distillation costs.

In the process presented in this work, the continuous recovery of the butanol is carried out by the flash fermentation technology (Mariano et al., 2008), in which the fermentor remains at atmospheric pressure and the broth is circulated to a vacuum chamber where butanol is continuously boiled off. Mathematical modeling was employed to analyze the process characteristics and to determine the best control structures.

2. Process description and mathematical modeling

Fig. 1 depicts the flash fermentation process, which consists of three interconnected units, as follows: fermentor, the cell retention system (tangential microfiltration) and vacuum flash vessel.

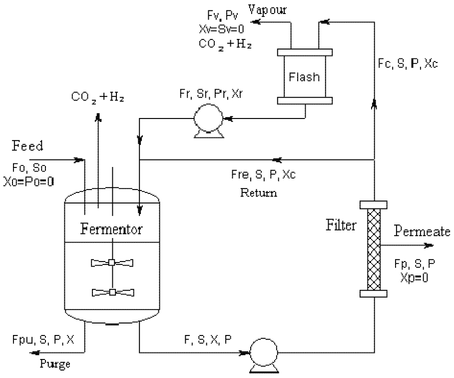


Fig. 1. Continuous flash fermentation process

The process starts as a conventional continuous fermentation until steady state is reached. Then, the flash tank separation system is turned on, where a partial separation of the solvents and water mixture occurs. The liquid fraction returns to the fermentor and the vapor fraction (after being condensed), added to the purge and permeate streams, will compose the final stream that is sent to distillation.

The study is carried out through computer simulation of a mathematical model based on experimental kinetic parameters (Mulchandani and Volesky, 1986), thus ensuring the physical meaning of the results.

Assuming constant volume, the mass balance equations for the continuous flash fermentation process are given by equations (1-4):

$$\frac{dX}{dt} = r_X - \frac{F_{PU}}{V} X \tag{1}$$

$$\frac{dS}{dt} = r_S + \frac{F_0}{V} S_0 - \frac{F_{PU}}{V} S - \frac{F_P}{V} S \tag{2}$$

$$\frac{dP_i}{dt} = r_{P_i} - \frac{F_{PU}}{V}P_i - \frac{F_P}{V}P_i - \frac{F_V}{V}P_{vi} \qquad (3)$$

where *i* stands for butanol, acetone, ethanol, butyric acid and acetic acid.

$$F_P = F_0 - F_{PU} - F_V \qquad (4)$$

The dynamics of the flash tank are much faster than that of the fermentation process, so a ‘pseudo’ steady state was assumed for the flash tank. The mass balance over the flash tank is given by Eq. (5).

$$Fc = F_V + F_r \qquad (5)$$

The modeling of the flash tank was based on the isothermal and isobaric evaporation model (Sandler, 1999) and a multicomponent system (water, butanol, acetone, ethanol, acetic acid and butyric acid) was considered. The vapour-liquid equilibrium of the mixture was calculated by Eq. (6); the value of P_i^{sat} was calculated by Antoine’s equation and the value of the activity coefficient (γ_i) by the UNIQUAC model.

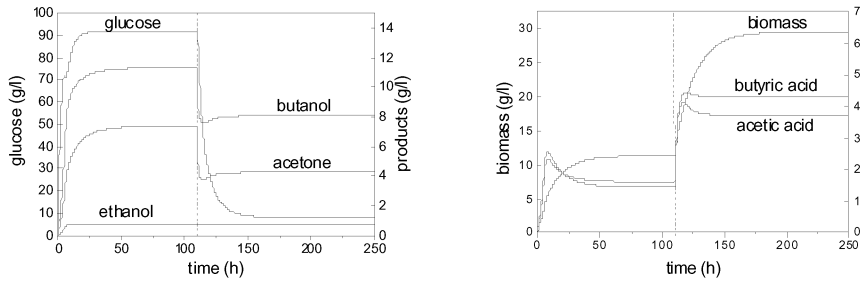
$$K_i = \frac{y_i}{x_i} = \gamma_i \frac{P_i^{sat}}{P} \qquad (6)$$

Eq. (1) to (6) were solved using a Fortran program with integration with an algorithm based on the fourth order Runge-Kutta method.

3. Process dynamics

Fig. 2 shows the dynamic behavior of the flash continuous fermentation process. When the flash system is switched on, significant changes in the process parameters are observed. The concentration of butanol in the fermentor lowers, which represents a significant reduction in the inhibitory effect, and, as a consequence, biomass concentration increases, resulting in a higher conversion of substrate. At this point, it is worthwhile stressing the benefits of the proposed process for ABE products with emphasis on the butanol: due to the continuous removal of the fermentor products, butanol concentration lowers and the cell activity increases.

The operating conditions considered for the ABE fermentation are listed in Table 1. An industrial-scale process was taken into account for the design.



(a) (b)

Fig. 2. Simulation results of glucose and products (a), and biomass and the intermediates (b).The vertical dashed line indicates the time when the flash tank separation system is turned on.

Table 1 Operating conditions of the continuous flash fermentation process

Parameter	Value	Unit
V	400	m^3
F_0	100	m^3/h
S_0	145	g/l
F_{pu}	25	m^3/h
F_c	400	m^3/h
T_{ferm}	37	°C
T_{flash}	37	°C
P_{flash}	6.5	kPa

The evaluation of the flash fermentation process performance with respect to butanol yield and productivity and sugar conversion is very important. This evaluation was obtained by a set of simulations, in which changes in the inlet substrate concentration were performed (Fig. 3). As the most attractive characteristic of the technologies for continuous butanol recovery from the fermentation broth is the increase in productivity by processing a concentrated feed stream, the range of the substrate concentration chosen (100–300 g/l) was considerably higher than the typical maximum concentration found in batch processes (60 g/l) (Ezeji et al., 2007).

Fig. 3 shows that with a variation in the substrate concentration of 100 to 150 g/l, the butanol yield achieves its maximum value of 20.5% and the butanol productivity increases from 4.51 to 7.70 g/l.h (for the operating conditions considered in Table 1). However, for the same substrate variation, the sugar conversion decreases from 98.5 to 92.9%. For concentrations above 150 g/l, yield and conversion decrease continuously and productivity is practically constant.

In our previous work (Mariano et al., 2008) the most relevant variables of the process (feed substrate concentration S_0, residence time, t_r, purge flow rate, F_{pu}, and the feed flow of the flash tank, F_c) were optimized, resulting in a butanol productivity of 9.2 g/l.h with a substrate conversion of 95%.

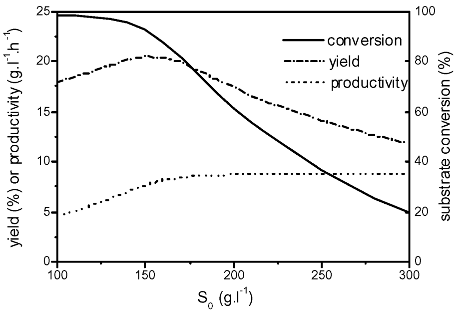


Fig. 3. Effect of sugar concentration on butanol yield and productivity and on sugar conversion for $F_0 = 100$ m^3/h, $tr = 4.0$ h, $Fpu = 25$ m^3/h, $Fc = 400$ m^3/h, $P_{flash} = 6.50$ kPa

The industrial operation of the flash fermentation process requires the development and implementation of an efficient control strategy, able to keep the main process variables in its set points in spite of load disturbances and/or set point changes. Thus, to choose the best control structures for the process, its open-loop dynamic behavior was investigated. The objective was to determine how the output variables are influenced by changes in the inputs (manipulated variables and possible disturbances). This was done by changing the values of the various input variables (one by one) and observing the change of the output variables with time.

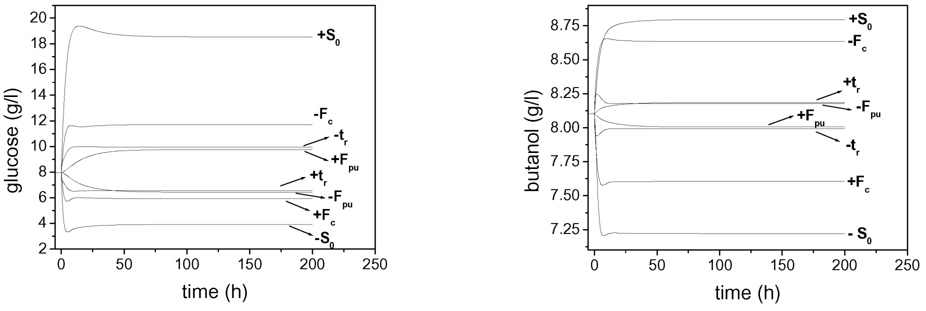
The outputs of the process are: biomass concentration in the fermentor (X), substrate concentration in the fermentor (S) and butanol concentration in the fermentor (P_{but}). The input variables considered for manipulation are: residence time (t_r), purge flow rate (F_{pu}) and the feed flow of the flash tank (F_c). The input variable considered as possible load disturbances is the inlet substrate concentration (S_0). In large scale fermentations, fluctuations in the quality of the raw material is constant, for instance the concentration of sugars in the sugar-cane depends on rainfall rates.

Fig. 4 shows the output variables (S, P_{but} and X) as functions of time after step perturbation of ±10% in the manipulated variables around the steady state (Table 1). Based on the responses of the process (magnitude of the variations), a table of the effects of the inputs on the outputs can be constructed. In Table 2, the grey area means that the input influences the output and the white area means that the influence is weak. This analysis can be used to determine the best structures for an efficient control of the process.

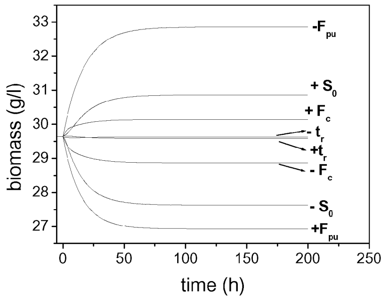
From Table 2 the following conclusions can be made: the biomass concentration can be controlled by the manipulation of F_{pu}; the best choice of manipulated variable to control the butanol concentration is F_c; substrate concentration (S) can be controlled by the manipulation of t_r; disturbances in S_0 have a strong influence on the output variables.

Table 2. Effects of the inputs on process outputs

	S_0	t_r	F_{pu}	F_c
X	▨		▨	
S	▨	▨	▨	▨
P_{but}	▨			▨



(a) (b)



(c)

Fig. 4. Dynamics of glucose (a), butanol (b), and biomass (c) concenstrations in the fermentor after step perturbations (±10%) in the manipulated variables.

4. Conclusions

Previous work shows that optimized process conditions make this process to be operated in very profitable ranges. The high level of productivity achieved by the flash fermentation is an important factor that can turn this process into a promising technology for the biobutanol industry. Moreover, with a final butanol concentration greater then 20 g/l, it is expected a meaningful reduction in the distillation costs and environmental benefits due to lower quantities of wastewater generated by the process.
Analyzes of the open-loop dynamic behavior of the process, after step perturbations in the manipulated variables, determined the best control structures for the process. Future works should focus on finding the best control algorithms for the process.

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References

Ezeji T.C., Qureshi N. and Blaschek H. P., 2007, Bioproduction of butanol from biomass: from genes to bioreactors, Curr. Op. Biotechnol., 18, 220-227.

Mariano A. P., Costa C. B. B., Angelis D. F., Maugeri Filho F., Atala D. I. P., Wolf Maciel M. R. and Maciel Filho R., 2008, Optimization Strategies Based on Sequential Quadratic Programming Applied for a Fermentation Process for Butanol Production, Appl. Bioch. Biotechnol., DOI 10.1007/s12010-008-8450-6.

Mulchandani A. and Volesky B., 1986, Modelling of the acetone-butanol fermentation with cell retention, Can. J. Chem. Eng., 64, 625-631.

Sandler S. I., 1999, Chemical & Engineering Thermodynamics. New York: John Wiley & Sons.