ADVANCED FEEDBACK-FEEDFORWARD CONTROL OF A TUBULAR REACTOR FOR A HIGH PRODUCTIVITY ETHANOL PROCESS: APPLICATION OF AN ALTERNATIVE STRUCTURED MODEL

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Abstract

Compared with growing studies of microorganism populations, few improvements on the development and application of structured models for product formation have appeared. This work presents an alternative dynamic structured model, adapted from a structured growth model and modified with the objective to simulate and to control a high productivity ethanol tower bioreactor. The original model of *Sacharomyces cerevisae* growth was adapted for ethanol production. Reduction techniques were applied in the particle direction and the reduced model was open loop simulated under disturbances in the inlet variables to define the control point and the manipulated variable. Because of the slow dynamic, it was necessary to establish, through "experimental planning", a relationship among the manipulated variable, the feed substrate concentration and a feedforward control strategy. The controller design involved a SISO form, the classic (PID), the advanced predictive (DMC) and the predictive adaptive (STDMC) control algorithms. A feedforward approach is proposed based on a statistical model. The reduction techniques were useful to obtain a structured model for applications in simulation and control. The study of control showed that an early action relating the manipulated variable and the set-point coupled to feedback control algorithms is the best form for promptly stabilize the process.

Keywords

Feedback-feedforward control, Reduction techniques, Bioreactor, Ethanol , Structured kinetic model.

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Introduction

Although unstructured models like Monod (1949), can be advantageously applied for the description of behaviour system, many important information are lost in such simplified approach. In the Harder and Roels (1982) there is a large number of applications in which these models fail. It applies, particularly, to transient situations such as: batches, fed batch or continuous culture or when the biomass composition changes drastically, like in some stages of the process and the early stages of batch growth (lag phenomena), and in situations where a specific constituent (e.g protein, RNA, Enzymes) must be modelled. Despite the complexity of the model, it matters that the structured model be as simple as possible. The class of the useful models is the ones where biomass is represented by two or three compartments, Harder and Roels, 1982.

In this work a simple structured growth model based on Rotboll and Jorgensen (1993) for batch and continuous culture was developed. The model was modified for a continuous type tower bioreactor by fitting the parameters related to the glycolysis and respiratory pathways with experimental data to represent the ethanol production process instead of growth, Stremel (2001). Such a model has both, structured biomass and structured metabolism, with oxidative and oxidoreductive mechanisms which promote growth, acetaldehyde and ethanol accumulation. Other characteristics are considered as inhibition by the ethanol accumulation and cell death rate

Open loop simulations have shown that the dynamic is very slow and for this reason it requires an anticipated action from the controller to provide faster answers. Different algorithms and control strategies were tested. A feedforward action was developed for the manipulated variable through statistical procedure. A central composite experimental design was applied for two factors, substrate and feed flow rate. A relationship was then obtained between ethanol as the dependent, and the two others as independent variables. Advanced control algorithms like DMC and adaptive DMC presented better performance when coupled to the statistical model.

Particle model

Biotic Phase

The substances considered for the biotic phase are those that diffuse through cell and particle (pellet) boundaries. In the eq. (1), the brackets depends on the substance, [A] is acetaldehyde, [P], Piruvate; [E], Ethanol and [S] is substrate The generic equation for the substances are given by equation (1).

$$\frac{\partial [\ ]}{\partial t} = \frac{D_{[\ ]}}{R_P^2}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial [\ ]}{\partial r}\right) \pm \nu_{[\ ]} \qquad (1)$$

Several reduction techniques were tested. Compared to the experimental data, was noted that both, reduced and not reduced form presented similar performances, Stremel et al (1999). In this paper, a classic reduction was applied in the Eqn. (01) to obtain a lumped model, Eqn. (2). Depending on the reduction technique utilized, modifications occur in the Bi_M^* term, Vasco de Toledo (1999) and Stremel (2001).

$$\frac{d[\ ]}{dt} = \frac{D_{[\ ]}}{R_p^2} 3Bi^*_{M[\ ]}\{[\ ]_f - \lambda[\ ]\} \pm \nu_{[\ ]} \qquad (2)$$

The boundary conditions are: symmetry at the center and resistance to mass transfer at the surface.

Reduction Techniques

The advantage to use reduction techniques is that the particle model reduces its complexity substantially, i.e it is possible to reconstruct the solution in the radial dimension, generating a lumped model from the distributed model.

Classic:

The classic reduction technique consists on to generate an average variable across a determined spatial direction. For the bioreactor this procedure is developed for the spherical geometry particle model . In this case, the mass modified Biot number, Cremasco (1998), has the same expression of that mass unmodified Biot number, Eqn.(4). Here, $D_{[\ ]}$ is the particle diffusion coefficient for each substance. The k_{TM} is the mass transfer coefficient, and R_P the internal particle ray. For the classic reduction, the λ= 1.

$$Bi^*_{M[\ ]} = Bi_{M[\ ]} = R_p k_{TM} / D_{[\ ]} \qquad (4)$$

Hermite *:*

This technique was not used in this work, it makes use of the approaches $H_{0,0}$, $H_{1,1}$ and simultaneously of the theorem mean value (classic reduction) for spherical co-ordinates. This becomes easier the generation of the radial medium variables, Vasco de Toledo (1999) and Stremel (2001).

In the approximation $H_{0,0}$, $Bi^*_{M[\ ]} = Bi_{M[\ ]}$ with $\lambda=2/3$

In the approximation $H_{1,1}$ is valid Eqn (5) with $\lambda=1$

$$Bi^*_{M[\ ]} = 4Bi_{M[\ ]} / \left(Bi_{M[\ ]} + 4\right) \qquad (5)$$

Abiotic Phase

The biomass compartments are divided into two parts: a synthetic compartment and a structural compartment. The concentration of synthetic compartment is Xs (g/gDW) that is responsible for the metabolic intermediates and enzymes. The concentration of structural/genetic

compartment is Xp (g/gDW); Xr (g/gDW) and X_f (g/gDW) are concentrations of respiratory and glycolytic enzymes. The last terms in the Eqn (6) to (9) accounts for the dilution of the abiotic state by the increase in X_t (gDW/L), the total biomass. The unit gDW is the cell dry weight in grams.

The abiotic compounds do not diffuse out of the pellet but they make part of the inner structure of the cell and they reflect the inside cell mechanism. From the Eqn. (6) to the Eqn. (10) with Eqn. (2) they express the lumped structured kinetic model. Eqn (10) was modified to consider inhibition by the ethanol accumulation and cell death rate.

$$\frac{dXs}{dt} = r_{Xs} - r_{Xp} - r_{Xr} - r_{Xf} - \left(r'_{Xs}\ Xs\right) \tag{6}$$

$$\frac{dXp}{dt} = r_{Xp} - \left(r'_{Xs}\ Xp\right) \tag{7}$$

$$\frac{dXr}{dt} = r_{Xr} - \left(r'_{Xs}\ Xr\right) \tag{8}$$

$$\frac{dXf}{dt} = r_{Xf} - \left(r'_{Xs}\ Xf\right) \tag{9}$$

$$\frac{dXt}{dt} = r'_{Xs}\ Xt\left(1 - \frac{Xt}{X_{SAT}}\right) e^{-K'_E\ [E]_f} - \left(k_d\ Xt\right) \tag{10}$$

Effectiveness Factor

It is known that the resistance of diffusion causes a concentration profile that exists in the pellet because reactants cannot diffuse from the bulk rapidly enough. The effectiveness, Eqn. (11) is defined as the global observed rate of flow through the pellet to the mean structured kinetic reaction term, Stremel (2001).

$$\eta_{[\ ]} = \frac{3\dfrac{D_{[\ ]}}{R_P^2}\dfrac{d[\ ]}{dr}\Big|_{r=1}}{\nu_{[\ ]}} \tag{11}$$

Applying the classic reduction technique, the effectiveness factor is given by the Eqn. (12)

$$\eta_{[\ ]} = 3\frac{D_{[\ ]}}{R_p{}^2} Bi^*_{M[\ ]} \frac{[\ ]_f - [\ ]}{\nu_{[\ ]}} \tag{12}$$

Fluid Phase Dynamic Model

The fluid phase model is based on an axial dispersed plug flow with a convective term taking into account dispersion, convective motion, and the mass transfer that is evaluated in terms of the effectiveness factor. The brackets, $[\ ]_f$ in Eqn. (13) are concentration of the substrate, ethanol, pyruvate and acetaldehyde compounds in the fluid phase. The $[A]_f$ and $[P]_f$ are intermediate compounds of the metabolic pathway which diffuse from the solid phase in low concentrations and make part of the structured metabolism. The $\nu_{[]}$ term is the mean structured kinetic reaction, which includes the stoichiometry of the metabolic network

$$\frac{\partial [\ ]_f}{\partial t} = \frac{D_{ax}}{L^2}\frac{\partial^2 [\ ]}{\partial z^2} - \frac{u}{L}\frac{\partial [\ ]_f}{\partial z} \pm \frac{1-\varepsilon}{\varepsilon}\eta_{[\ ]}\nu_{[\ ]} \tag{13}$$

Boundary Conditions

For the fluid phase, the boundary conditions are given by "Danckwerts conditions" (Froment and Bishoff, 1990). A correlation for the axial dispersion coefficient was adjusted with experimental data, Stremel (2001).

General Consideration for the Bioreactor Control Design

Control of physiological state of cells is often desired to stimulate their activity in a favorable direction. These control variables to be controlled are difficult to measure; therefore, a mathematical model must be used in some way to estimate the state of the process.

Difficulty in feedback control is twofold. Firstly, difficulties appear for the process to reach a new steady state. Under open loop flow rate disturbance, the time response of the process is slow. The control problems can arise because of severe non-linear behavior, which can lead to a long time process adaptation. Although sensors and feedback controllers have fast response quickly, the nature of the process is slow.

Secondly, a continuous process with immobilized cells many present problems of stability. When experimental procedure is conducted without a control for long time operation, ethanol concentration accumulates, and above certain limit (higher than 80g/L) it leads to the collapse of the process. After a period of operation, the recovery of the production is not possible and the process has to be re established with a new cell culture. These perplexities dictate the need for continuous monitoring and to readjusting the control strategy, to be able to establish the process promptly.

To improve the quality of control during the transient response a feedforward model was obtained through a central composite experimental planning, Stremel (2001). The statistical analysis was used to obtain the empirical equation that describes the ethanol production as function of substrate concentration and feed flow rate (feedforward model).

Through open loop simulations under disturbances, it was verified that the bioreactor exit was important to measure the ethanol concentration and to control the process. Because the limitation on the manipulated

variables, only a SISO configuration is possible to ensure the stability of the operation with high productivity, in these case, through manipulation of the feed flow rate.

Feedback-Feedforward Model

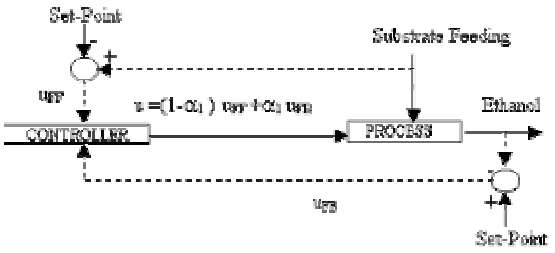

Figure 1: Feedback-Feedforward configuration

Figure 1 show the strategy considered for Feedback - Feedforward model configuration. The parameters were adjusted empirically after calculations under open loop simulations with set-point perturbation. The Feedback (DMC or PID) with a Feedforward model acts on the manipulated variable depending on the value of the parameter α_1. The optimised parameter of α_1 for both controls acting simultaneously is 0.2. For DMC, the parameter α is related to the behavior forced by the reference trajectory and λ is the moving suppressing factor, (Vasco de Toledo, 1999).

In Figure 2 it can be seen a comparison of the controller performances. The classic PID coupled and no coupled with a feedforward model had a good performance, although, DMC with feedforward model showed a superior performance than PID, when it was compared in terms of the manipulated variable profiles, depicted in Figure 3.

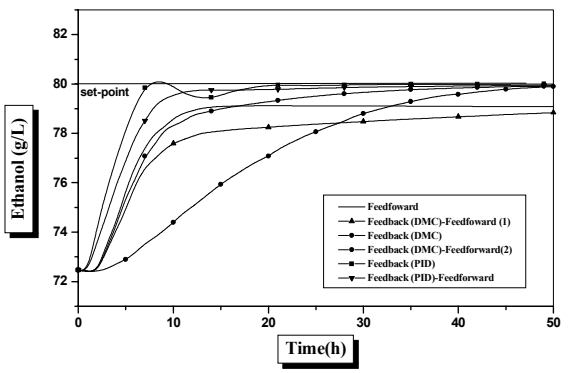

Figure 2: Control of the bioreactor considering set-point changing of 72,5 g/L to 80 g/L.

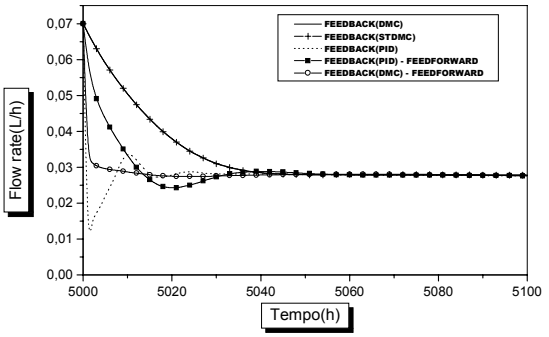

Figure 3: Manipulated variable profile for a closed loop simulation after a long steady state condition.

The Feedforward model obtained for the flow rate, manipulate variable (F), is given by the Eqn (14). The variables S_0 and $E_{f,sp}$ are the feed substrate concentration and the desired ethanol concentration (set-point), respectively .

$$F = \frac{-\left[-641.4 - (6.25x10^{-5} S_0)\right] - \sqrt{\Delta}}{4659.2} \qquad (14)$$

where:

$$\Delta = 25208.8 - 355.12 S_0 + 0.5908 S_0^2 + 9318.4 * E_{f,sp} \qquad (15)$$

Conclusions

The study of control showed that an early action relating the manipulated variable and the set-point (feedforward) coupled to algorithms of feedback control is the best form for quickly stabilizing the process.

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