Simulation of Fermentation Bioreactor Control for Ethanol Production

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Abstract — Today's concerning about global warming and the rapid depletion of coal, gas and crude oil reserves enforced the study of alternative fuels as bioethanol. Bioethanol can be blended at low concentrations with gasoline or diesel for use in today's vehicles, and is considered to be a sustainable transportation fuel. Present paper deals with aspects regarding the simulation of fermentation bioreactor process and fermentation bioreactor control for ethanol production. The bioreactor model was implemented in Matlab Simulink and the results of simulation using different control strategies are presented comparatively.

Index Terms — bioethanol production, continuous fermentation bioreactor, bioreactor modeling and simulation, bioreactor control.

I. INTRODUCTION

The main motivation for investments in research and process development concerning bioethanol production is environmental concern related to global warming. The focus is, in particular, turned towards the reduction of CO_2 emissions and other green house gases. Moreover, bioethanol production would decrease the dependency on the natural oil reserves, which can due to their restricted geographical localization cause political tension and economical instability.

Bioethanol can be blended at low concentrations with gasoline (usually 10% ethanol and 90% gasoline) or diesel for use in today's vehicles without engines modifications and without affecting vehicle warranty, and is considered to be a sustainable transportation fuel. Alternatively, if bioethanol is used in higher, or 100 % concentrations, but in this case adopted vehicles engines are typically needed.

Starting with biomass harvesting, there are a number of steps to follow until the final product, the ethanol is obtain(figure 1).



Fig. 1. Steps in bioethanol production.

Of these processes, present paper is studying the alcoholic fermentation of glucose to ethanol. The bioreactor in which the glucose fermentation takes place is a continuous stirredtank reactor with constant substrate feed flow. The three main components of the bioreactor are[2]:

- the biomass as a suspension of yeast fed into the system and evacuated continuously;
- the substrate which is solution of glucose needed in order to feed the micro-organism;
- ethanol as final product evacuated together with other components.

Inorganic salts, which are necessary compounds for the formation of coenzymes, are added together with the yeast.

II. BIOREACTOR MODEL

The kinetic equation used in the bioreactor model represents the Monod modified equations based on Michaelis-Menten kinetics, proposed by Aiba et al., and described by Z.K. Nagy[2-4].

The mass balances for the biomass is expressed by equation (1) as:

$$\frac{\mathrm{d}\mathbf{c}_{\mathrm{x}}}{\mathrm{d}\mathbf{t}} = \boldsymbol{\mu}_{\mathrm{x}} \mathbf{c}_{\mathrm{x}} \frac{\mathbf{c}_{\mathrm{s}}}{\mathbf{K}_{\mathrm{s}} + \mathbf{c}_{\mathrm{s}}} \mathrm{e}^{-\mathbf{K}_{\mathrm{p}}\mathbf{c}_{\mathrm{F}}} - \frac{\mathbf{F}_{\mathrm{e}}}{\mathbf{V}} \mathbf{c}_{\mathrm{x}} \tag{1}$$

where c_x represent the biomass(yeast) concentration(h⁻¹), μ_x is the maximum specific growth rate(h⁻¹), c_s is the glucose concentration(g/l), K_s is constant in the substrate term for growth(g/l), K_p represent constant of growth inhibition by ethanol(g/l), c_P is the product concentration (g/l), F_e is the outlet flow from the reactor(lh⁻¹), V is the volume of the mass of reaction(l).

The mass balance for product is obtain as[2]:

$$\frac{\mathrm{d}\mathbf{c}_{p}}{\mathrm{d}t} = \mu_{p} \mathbf{c}_{\mathrm{X}} \frac{\mathbf{c}_{\mathrm{S}}}{\mathbf{K}_{\mathrm{S}1} + \mathbf{c}_{\mathrm{S}}} \mathbf{e}^{-\mathbf{K}_{\mathrm{F}1} \mathbf{c}_{\mathrm{F}}} - \frac{\mathbf{F}_{\mathrm{e}}}{\mathbf{V}} \mathbf{c}_{\mathrm{p}} \tag{2}$$

where μ_P represent the maximum specific fermentation rate(h⁻¹), K_{S1} is the constant in the substrate term for ethanol production(g/l) and K_{P1} is the constant of fermentation inhibition by ethanol(g/l).

Equation (3) represent the mass balance for the substrate:

$$\frac{\mathrm{d}\mathbf{c}_{\mathrm{S}}}{\mathrm{d}\mathbf{t}} = -\frac{1}{\mathrm{R}_{\mathrm{SX}}}\frac{\mathrm{d}\mathbf{c}_{\mathrm{X}}}{\mathrm{d}\mathbf{t}} - \frac{1}{\mathrm{R}_{\mathrm{SP}}}\frac{\mathrm{d}\mathbf{c}_{\mathrm{p}}}{\mathrm{d}\mathbf{t}} + \frac{\mathrm{F}_{\mathrm{i}}}{\mathrm{V}}\mathrm{c}_{\mathrm{S,in}} - \frac{\mathrm{F}_{\mathrm{e}}}{\mathrm{V}}\mathrm{c}_{\mathrm{S}}$$
(3)

where R_{SX} is ratio of cell produced per glucose consumed for growth, R_{SP} is the ratio of ethanol produced per glucose consumed for fermentation, and $c_{S,in}$ represent the glucose concentration in the feed flow.

For the reactor and jacket, the energy balance is described

 $r_{\rm O} \Delta H_{\rm e}$

by equations (4) and (5)[2]. In this equations, T_{in} is the temperature of the substrate flow into the reactor(⁰C), T_r represent the temperature in the reactor(⁰C), r_{O2} is the rate of oxygen consumption(mgl⁻¹h⁻¹), ΔH_r is the reaction heat generated by the fermentation process, ρ_r and ρ_{ag} is the density of the mass of reaction respectively the density of cooling agent(g/l).

E.

represents the concentration of acid and base.

Equations (8), (10) and (11) correspond to the pH neutralization model, and this model is implemented in Simulink.

III. IMPLEMENTATION OF BIOREACTOR MODEL

The implementation of bioreactor model using Matlab Şimulink is presented in figure 2.

$$\frac{dT_{r}}{dt} = \frac{T_{r}}{V} (T_{in} + 273) - \frac{T_{r}}{V} (T_{r} + 273) + \frac{G_{2}}{32\rho_{r}C_{heat,r}} + \frac{T_{r}}{V\rho_{r}}$$
$$\frac{dT_{ag}}{dt} = \frac{F_{ag}}{V_{j}} (T_{in,ag} - T_{ag}) + \frac{K_{T}A_{T}(T_{r} - T_{ag})}{V_{j}\rho_{ag}C_{heat,ag}}$$
(5)

Also in the equations (4) and (5), K_T represent the heat transfer coefficient($Jh^{-1}m^{-2}K^{-1}$), A_T is the heat transfer area(m^2) and $C_{heat,ag}$ respectively $C_{heat,r}$ are the heat capacity of cooling agent and of mass of reaction($Jg^{-1}K^{-1}$).

The rate of oxygen consumption is[2]:

dT.

Π.

$$r_{o_2} = \mu_{o_2} \frac{1}{Y_0} c_X \frac{c_{o_2}}{K_{o_2 + c_{o_2}}} \tag{6}$$

with μ_{O2} maximum specific oxygen consumption rate(h⁻¹), K_{O2} constant of oxygen consumption(g/l) and c_{O2} oxygen concentration in the liquid phase(mg/l).

The balance for total volume for reaction medium is:

$$\frac{dV}{dt} = F_i - F_c \tag{7}$$

Regarding the model for pH neutralization process, it is known that the pH denotes the concentration of the ions $[H^+]$ through the following logarithmic function:

$$pH = -log_{10}[H^+]$$
 (8)

The dissociation equation for water is expressed as:

$$[H^+][OH^-] = K_w = 10^{-14}$$

and K_w can be express as [7]:

$$\begin{bmatrix} H^{+} \end{bmatrix} = \frac{X}{2} \left(\sqrt{1 + \frac{4K_{w}}{X^{2}}} - 1 \right) & \text{if } X > 0 \\ \begin{bmatrix} H^{+} \end{bmatrix} = \frac{X}{2} \left(\sqrt{1 + \frac{4K_{w}}{X^{2}}} + 1 \right) & \text{if } X < 0 \quad (10) \\ \begin{bmatrix} H^{+} \end{bmatrix} = \sqrt{K_{w}} & \text{if } X = 0 \end{bmatrix}$$

The equation describing the pH neutralization process dynamics is[5-7]:

$$V\frac{dX}{dt} = c_{B}F_{B} - c_{A}F_{A} - (F_{A} + F_{B})X$$
(11)

where F_A and F_B are the flow of acid and base, c_A and c_B



Each of the equations describing the model was implemented using Function Blocks from Simulink.

Some of the parameters can be modified as one can see in figure 3.

🛃 Function Block Parameters: S	Subsystem2
MODELUL BIOREACTORULUI	CONTINUU CU AMESTECARE MECANICA (mask)
This model was developed un advanced technology-PRODOC 2008/2011.	nder "Project for development of doctoral studies in C" in Technical University of Cluj-Napoca, between
Copyright 2008-2011 MARGIN	EAN Ana-Maria Claudia
Parameters	
Bioreactor volumei [I]	
1000	
pH-ul in pH units	
the second s	
6	
6 Temperature of cooling agent	t when enteriing in the cooling jacket in degree Celsius
6 Temperature of cooling agent	t when entering in the cooling jacket in degree Celsius
6 Temperature of cooling agent 15 Quantity of NaCl in grams	t when entering in the cooling jacket in degree Celsius
6 Temperature of cooling agent 15 Quantity of NaCl in grams 500	t when entering in the cooling jacket in degree Celsius
6 Temperature of cooling agent 15 Quantity of NaCl in grams 500 Quantity of CaCO3 in grams	t when enterling in the cooling jacket in degree Celsius
6 Temperature of cooling agent 15 Quantity of NaCl in grams 500 Quantity of CaCO3 in grams 100	t when entering in the cooling jacket in degree Celsius
6 Temperature of cooling agent 15 Quantity of NaCl in grams 500 Quantity of CaCO3 in grams 100 Quantity of MgCl2 in grams	t when entering in the cooling jacket in degree Celsius

Fig. 3. Block for parameter input

Because the temperature in the reactor depends of the flow of cooling agent, the first step in our analysis was to apply a step change in the flow of cooling agent in order to study the influence on the reactor temperature. The applied step change and the evolution of the temperature in the reactor are depicted in figure 4.



Fig. 4. Step change and the reactor temperature evolution In order to study the dynamic behavior of the bioreactor

(9)

system a step change with 2° C in inlet flow temperature was applied, which can occur due to the ambient temperature[2]. The results are presented in figure 5.



Fig. 5. Dynamic response of the bioreactor in the case of step change in the temperature input flow

Analyzing the results of the simulation, one can observe that the effect of the change in the inlet temperature have a major impact on the ethanol concentration and can be considered as a major disturbance in the system.

The implementation of the pH neutralization model is presented in figure 6.



Fig. 6. Model for pH neutralization process

The model was implemented using equations (8), (10) and (11) as is presented in figure 7. In order to study the response of the implemented model, a step change in the flow of base was simulated. The step change and the evolution of pH are presented in figure 8.



Fig. 7. Implementation of pH neutralization process models



Fig. 8. Step change and the pH evolution

A step change in the flow of base increases the pH value demonstrating that the implemented model can be used in our study.

IV. CONTROL STRATEGIES

Two control strategy has been take into account, based on simple bi-positional controller and PID controller.

The used PID controllers from Simulink have the possibility of tuning. and optimal PID controllers parameters was obtained.

The results of simulations for different control strategies using pH neutralization models are presented in figure 9.



Fig. 9. Comparative results for pH control

For the bioreactor implemented model, the results using different control strategies are presented in figure 10.

V. CONCLUSION

Models for bioreactor used in glucose fermentations and for pH neutralization process are presented. The models was implemented using Matlab Simulink and different control strategies are studied. The results of the study are presented comparatively in this paper. The study will continue with the implementation of different control strategies, in order to find optimal control strategy for temperature and pH.



Fig. 10. Comparative results for bioreactor temperature

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