Simulation and control of fermentation complex systems

D. Chmúrny, R. Chmúrny

Abstract The paper deals with biotechnological complex systems with focus onto fermentation processes. Discontinuous, semicontinuous and continuous fermentation processes are discussed. Mathematical model of continuous biotechnological process for ethanol production is introduced and verified.

1 Introduction
Many fermentation processes are commonly used today, but their effective control is not yet fully handled. The following factors prevent the full use of modern control methods:

- Limited availability of process analysers and real-time measuring methods of those biological and physico-chemical parameters, which are required for instant determination of fermentation process state.
- Limited possibilities of interpretation of obtained information in a form directly applicable for closed loop control process synthesis.
- Insufficient number of effective identification and control methods which would be appropriate for real-time operation of the computer-fermentor system.

2 Problem formulation
Fermentation, which is based on growing of microbial cultures at the expense of consumption of carbonaceous substrates, is realized in fermentors. This biotechnological process is oriented either to the production of cellulosic cellular mass (proteins, endoxins, etc.), either to the production of organic substrates resulted from the metabolic activity of micro-organisms (antibiotics, alcohols, etc.) or to extraction of some components of nutritious liquids.

In generally three types of fermentation are used:
1. Discontinuous fermentation
2. Semicontinuous fermentation
3. Continuous fermentation

Discontinuous fermentation is performed in a closed reactor in advance filled with the substrate and inoculated by micro-organisms. Process, when the fermentor is permanently supplied with the substrate and at the same time the products are extracted, is called continuous fermentation. Semicontinuous fermentation is characterised by periodic injection of substrate.

3 Basis of constructing mathematical models of biotechnological processes
Stationary biotechnological process with lumped parameters can be described as system of differential equations in the following form:

\[ \frac{dx}{dt} = f(x(t), u(t), \mathbf{p}) \]  

where \( x \) is the vector of state variables, \( u \) is the vector of control variables, \( \mathbf{p} \) is the vector of model parameters.

Mathematical models of biotechnological processes are as a rule nonlinear. In the process of forming these models a sequence of simplification steps has to be made. Majority of papers dealing with the construction of fermentation models are based on setting up of process kinetic equations. Material and energetic balances are very often used too. For deriving of such balances the model of micro-organisms activity must be clearly understood. A micro-organism consumes certain substrates (oxygen, nitrogen, hydrocarbons), which are then transformed into biosubstance as products (ethanol, glucic acid, penicillin etc.) and metabolites (water, carbon dioxide, etc.). Basic stoichiometric equation of balance, on whose base the static and dynamical mathematical models are formulated, has the following form:

\[ a \cdot C_xH_yO_z + b \cdot O_2 + c \cdot NH_3 \rightarrow d \cdot C_yH_bO_yN_n + e \cdot H_2O + f \cdot CO_2 + Q_R \]  

where \( a, b, c, d, e, f \) is the number of mols of reagents and of products, \( C_xH_yO_z \) is the substrate, \( C_yH_bO_yN_n \) is the product and \( Q_R \) is heat.

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D. Chmúrny
Department of Automation, Faculty of Chemical Technology, Slovak Technical University, Radlinského 9, SK-812 37 Bratislava, Slovak Republic

R. Chmúrny
Institute of Materials and Machine Mechanics, Slovak Academy of Sciences, Račianska 75, SK-838 12 Bratislava 38, Slovak Republic

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4 Mathematical modelling of discontinuous and semicontinuous biotechnological processes

Different fermentation flow charts are depicted in Figs. 1 and 2. In these figures the following notation is used: $F$ is volume velocity of dosing of refilling substrate (m$^3$·h$^{-1}$); $V$ is the instant volume of the fermenter contents (m$^3$); $x, s$ are concentration of the biomass and of the substrate, respectively (g·l$^{-1}$); $x_{HI}, s_{HI}$ are initial concentration of biomass and substrate (g·l$^{-1}$); $V_{HI}$ is initial volume of fermentor (m$^3$); $P$ is concentration of the final product (g·l$^{-1}$); $x, s$ are concentrations of the biomass and of the substrate, respectively (g·l$^{-1}$); $s_0$ is concentration of substrate in refilling solution (g·l$^{-1}$), and $V_N$ is volume of refilling substrate (m$^3$).

In the fermentor a complex process of microbiological synthesis is running, which is influenced by various internal and external factors. The process in fermentor is considered as stationary and deterministic. Also ideal mixing of all substances present in the reactor is assumed.

Let us denote $\mathbf{u} = [\mathbf{u}', \mathbf{u}'']$ as the vector containing all control quantities which have influence on the fermentation process so as:

$$\mathbf{u}' = [T, pH, C_{O_2}, \cdots]^T, \quad \mathbf{u}'' = [D, F, s_0]^T = [u_1, u_2, u_3]^T,$$

where $T$ is temperature of fermentation contents ($^\circ$C), $C_{O_2}$ is concentration of dissolved oxygen in fermentor ($\%$), $F = dV/dt$ is the flow rate and $D = F/V$ is the rate of control.

The general mathematical model of semicontinuous fermentation process has the following form:

$$\frac{dx}{dt} = \mu(x, s, \mathbf{u}')x - \frac{u_2}{V}x,$$

$$\frac{ds}{dt} = -\eta(x, s, \mathbf{u}')s + \frac{u_2}{V}(s_0 - s),$$

(3)

Fig. 1. Discontinuous fermentation process.

$t = 0, x \approx 0; s = s_{HI} = s_{max}; P = 0; V = V_{HI} = \text{const.}$

$t = t_k, x = s_{HI}; s \rightarrow 0; P = P_k, V = \text{const.}$

The observed law of the discrete process depicted in Fig. 2 is as follows:

$$\frac{dx}{dt} = \mu(x, s, P, \mathbf{u}')x - u_1 x_1,$$

$$\begin{align*}
\left\{ \text{rate of biomass concentration} \right\} &= \left\{ \text{rate of biomass discharge} \right\} + \left\{ \text{change caused by exponential growth} \right\}, \\
\left\{ \text{rate of biomass discharge} \right\} &= \left\{ \text{change caused by exponential growth} \right\}.
\end{align*}$$

(4)

Fig. 2. Semicontinuous fermentation process.

$t = 0, x \approx 0; s = s_{HI}; P = 0; V = V_{HI},$

$t = t_k, x = s_{HI}; s \rightarrow 0; P = P_k; V = V_{HI} = V_{HI} + V_N$

$$\frac{dP}{dt} = \ell(x, s, \mathbf{u}')x - \frac{u_2}{V}P,$$

$$\frac{dV}{dt} = u_2,$$

where $\mu, \eta, \ell$ are relative velocities of biomass growth, substrate consumption and final product growth, respectively.

For discontinuous process the same mathematical model, Eq. (3), can be used with $u_2 = 0$.

5 Mathematical modelling of continuous biotechnological processes

Development of science and the opportunity of better utilisation of control methods in biotechnology made possible to replace discontinuous processes by continuous ones. The advantages of continuous processes is that micro-organism growth is more effective and controllable, because a steady equilibrium growing mode can be achieved. In a continuous process the fermentation must be interrupted and restarted again, and due to this way of operation the conditions vary, which unfavourably influences the micro-organism growth and also output product steady quality. A scheme of continuous biotechnological process is depicted in Fig. 3.

The water and supplementing substrate are injected into the fermentor and from the collector the culture is discharged at the same rate $F_2$ (m$^3$·h$^{-1}$) so as the volume of fermenter contents $V$ is held constant. The aim is to keep the temperature and pH on constant value, while the rate of micro-organism growth is determined by the rate of control $D = F_3/V$ and by concentration of supplementing substrate $s_0$. Variation of concentration $s_0$ is achieved by water supply rate $F_1$ (m$^3$·h$^{-1}$).

The general mathematical model of continuous biotechnological process has the following form:

Biomass balance:

$$\frac{dx}{dt} = \mu(x, s, P, \mathbf{u}')x - u_1 x_1,$$

$$\left\{ \text{rate of biomass concentration} \right\} = \left\{ \text{rate of biomass discharge} \right\} + \left\{ \text{change caused by exponential growth} \right\},$$

(5)

Fig. 3. Continuous fermentation process. W-water, S-supplementing substrate. $0 \leq t \leq t_0, x = x_0 = \text{const.}; P = P_0 = \text{const.;} S = S_0 = \text{const.;} V = \text{const}$