SOME RESULTS REGARDING NUMERICAL MODELLING AND SIMULATION OF A FERMENTATION PROCESS

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1. INTRODUCTION

Biotechnical processes and especially the fermentation ones had known in the last few years, an ample developing and a remarkable past progress worldwide and also at national level. A distinct interest can be remarked from the control and optimization of fermentation processes with numerical calculator help. A determinative role played by the construction of the model, the identification of the process, the estimation of the parameters and the analysis of the model.

The fermentation processes have some specific features, such as:

- they generally have a discontinuous character (of charge) because of limited lifetime of the micro organisms;
- they are variable in time, because they depend on micro organism's biological activity, specific to every charge;
- they are characterized by powerful interdependence between parameters and by important unliniarities (multivariable and unliniar process);

The major difficulties in the atomisation of these processes appear because of the available measurement and control devices and because of the insufficient knowledge of the process dynamic.

2. MATHEMATICAL MODELS OF THE FERMENTATION PROCESSES

Fermentation represents the growing process of the micro organisms by different cultures for biosynthesise products. The growing of the micro organisms is regarded in terms of the cellular mass, cellular density or micro organisms number, respectively of the cellular concentration.

The important quantities that concern these systems are: the total biomass, the organic substrate, the dissolved oxygen and the final product. In some cases it is necessary to take care of other quantities too, like: phosphorus, nitrogen, and temperature that depend on the specific conditions of the studied process.

The basic structure of a fermentation device model in continuous flux with concentrates parameters can be written as:

$$\frac{dX(t)}{dt} = \sum_i D_i(t)X_i(t) - D(t)X(t) + \mu(t)X(t) - K_D X(t) \quad (1)$$

$$\frac{dS(t)}{dt} = \sum_i D_i(t)S_i(t) - D(t)S(t) - \frac{1}{Y}\mu(t)X(t) \quad (2)$$

$$\frac{dC(t)}{dt} = \sum_i D_i(t)C_i(t) - D(t)C(t) + K_{La}(F_A(t))[C_S(t) - C(t)] - O_2C(t) \quad (3)$$

$$\frac{dP(t)}{dt} = \sum_i D_i(t)P_i(t) - D(t)P(t) + [Y_{P/X}\mu(t) + \beta(\mu(t) - d(X(t), P(t)))]X(t) \quad (4)$$

where:

X – the active biomass concentration
S – the organic substrate concentration
C – the dissolved oxygen concentration
P – the final product concentration
D_i represents different alimentation flows
K_D – the old age organism constant
Y and $Y_{P/X}$ – are the crop coefficients
K_{La} – the oxygen transfer speed
F_A – the airflow speed
C_S – the oxygen saturation concentration
$\mu(t)$ – the growing specific speed of biomass that verifies so-called expression modified Monod.

$$\mu(t) = \frac{\mu_m S(t)}{K_S + S(t)} \cdot \frac{C(t)}{K_C + C(t)} \quad (5)$$

where μ_m and K_S are constants and O_2C is the oxygen speed that is in relation with the growing and maintenance of the breathing.

$$O_2C(t) = a\mu(t)X(t) + bX(t) \quad (6)$$

where "a" and "b" are constants.

Thermal balance equation:

$$\frac{dT(t)}{dt} = K_D O_2 C(t) - q_r A(T(t) - T_r) \qquad (7)$$

where T_r – cooling fluid temperature, and q_r and A are proportionality coefficients.

3. EXPERIMENTAL RESULTS

It was considered an open and homogeneous fermentation process with aerobes cultures fixed in a fermentation device that present oxygen excess. The single model limitation has been considered the substrate concentration.

The differential equations of the considered model are:

$$\frac{dX(t)}{dt} = (\mu(t) - D)X(t) \qquad (8)$$

$$\frac{dS(t)}{dt} = F - DS(t) - \frac{\mu(t)X(t)}{Y_c} - m_c X(t) \qquad (9)$$

where: X(t) = active biomass concentration (of the dregs)

S(t) = the concentration of the carbon substrate

D = the replacement speed per hour of the fermentation device or the dilution rate

F = the alimentation rate with substrate

m_c = the substrate consuming rate because of the growing rate

Y_c = the efficiency of the cellular mass accumulation

$$R_c = -\frac{\mu(t)X(t)}{-\frac{\mu(t)X(t)}{Y_c} - m_c X(t)} = \frac{\mu(t)}{m_c + \frac{\mu(t)}{Y_c}} \qquad (10)$$

represent the biologic global production.

Using for μ(t) an expression like (5) it was obtained unsatisfactory results. Consequently we made use of a relation that effectively take care of that part of S(t) noted with S^* who contribute to the growing.

$$S^*(t) = \frac{S \cdot S_{sat}}{S + S_{sat}} \qquad (11)$$

That led us to the expression

$$\mu(t) = \mu_m \frac{1}{\frac{A_1 X(t)[S(t) + S_{sat}]}{S(t) S_{sat}} + 1} \qquad (12)$$

using the notations: $X(t) = X_1(t)$; $S(t) = X_2(t)$; $\mu_m = p_1$; $Y_c = p_2$; $A_1 = p_3$; $m_c = p_4$; $S_{sat} = p_5$ and adopting the vectors notations will obtain:

$\underline{Y}^T = [X_1, X_2]$ state vector; $\underline{U}^T = [D, F]$ control vector;

$\underline{p}^T = [p_1, p_2, p_3, p_4, p_5]$ parameters vector

$$\dot{\underline{Y}} = \frac{d\underline{Y}}{dt} = \begin{bmatrix} \frac{dX_1}{dt} \\ \frac{dX_2}{dt} \end{bmatrix}$$

The parameters identification was made by simulation using the sensibility functions method.

The following optimisation criterion was used:

$$I = \sum_{k=1}^{N} \left[\left(X_1^k - \hat{X}_1^k \right)^2 + \left(X_2^k - \hat{X}_2^k \right)^2 \right] \qquad (13)$$

where $\hat{X}_1^k$ and $\hat{X}_2^k$ represent the measured dates.

The criterion function has been derived with respect to the system parameters, obtaining:

$$\frac{\partial I}{\partial p_i} = -2 \sum_{k=1}^{N} \left[\left(X_1^k - \hat{X}_1^k \right) \frac{\partial \hat{X}_1^k}{\partial p_i} + \left(X_2^k - \hat{X}_2^k \right) \frac{\partial \hat{X}_1^k}{\partial p_i} \right] \qquad (14)$$

where i = 1, 2, …, 5.

The sensibility functions of the state variables were noted with:

$$s_{11} = \frac{\partial X_1}{\partial p_1}; \quad s_{12} = \frac{\partial X_1}{\partial p_2} \ldots\ldots \quad s_{15} = \frac{\partial X_1}{\partial p_5}$$

$$s_{21} = \frac{\partial X_2}{\partial p_1}; \quad s_{22} = \frac{\partial X_2}{\partial p_2} \ldots\ldots \quad s_{25} = \frac{\partial X_2}{\partial X_5}$$

and $\frac{dS_{ij}}{dt} = \frac{\partial}{\partial pj}\left(\frac{\partial X_i}{\partial t}\right)$ and $s\mu_{pj} = \frac{\partial \mu}{\partial pj}$

i,j=1, 2, …, 5.

The model parameters were determined minimizing the criterion function.

In stationary conditions we will obtain the equations:

$$\left[\frac{p_1 p_5 X_2}{X_2(p_3 X_1 + p_5) + p_5 X_1} - D\right] X_1 = 0 \quad (15)$$

$$F - DX_2 - \frac{p_1 p_5 X_1 X_2}{p_2\left[X_2(p_3 X_1 + p_5) + p_5 X_1\right]} - p_4 X_1 = 0 \quad (16)$$

Solving the system formed with equations (15) and (16) two stationary regimes will be obtained:

$$X_{1s}^1 = 7{,}2598586$$
$$X_{2s}^1 = 5{,}8793325 \quad (17)$$

$$X_{1s}^2 = 39{,}290031$$
$$X_{2s}^2 = -65{,}7729190 \quad (18)$$

The system (17) constitutes the real and physical feasible solution of the process. For numerical simulation the identification values of the parameters were considered: $p_1 = 0{,}212$; $p_2 = 1{,}428$; $p_3 = 0{,}087$; $p_4 = 0{,}123$; $p_5 = 1{,}521$ and like initials values $X_{10} = 6$g/l; $X_{20} = 10$g/l.

The computer simulation results for the case of the discontinuous process are presented in fig.1, and for the case of the continuous flow process in table 1 and fig.2. Analysing the obtained results comparing with measured dates we can say that the presented model describe accurately enough the fermentation process concerned.

Table 1.

Time	*CALCULATED VALUES*				*MEASURED VALUES*	
	X_1[g/l]	X_2[g/l]	μ	R_c	X_1[g/l]	X_2[g/l]
0	6,165	9,846	0,1458	0,648	6,173	9,921
5	8,184	7,421	0,1323	0,713	8,203	7,329
10	10,21	4,37	0,1717	0,871	10,22	4,375
15	11,2	1,26	0,0854	0,971	11,31	1,262
20	10,7	0,427	0,0537	0,934	10,72	0,512
25	9,71	0,673	0,0697	0,856	9,721	0,671
30	9,45	0,847	0,0779	0,859	9,45	0,842
35	9,43	0,915	0,0805	0,849	9,432	0,913
40	9,46	0,919	0,0806	0,853	9,457	0,920
45	9,48	0,901	0,0802	0,858	9,48	0,907
50	9,49	0,903	0,08	0,860	9,492	0,907
55	9,49	0,903	0,08	0,860	9,492	0,907
60	9,49	0,903	0,08	0,860	9,492	0,907

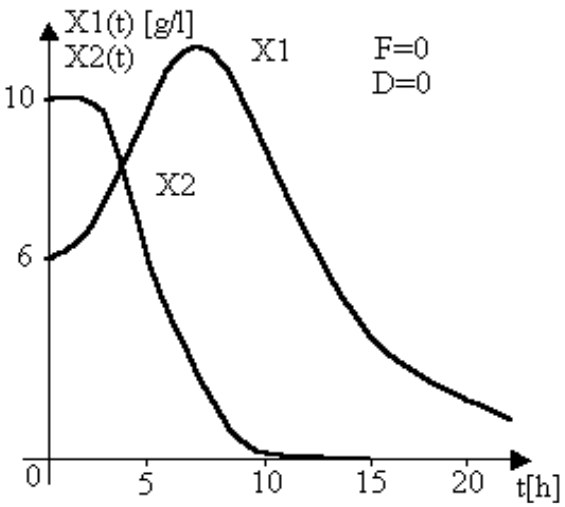

Figure 1.

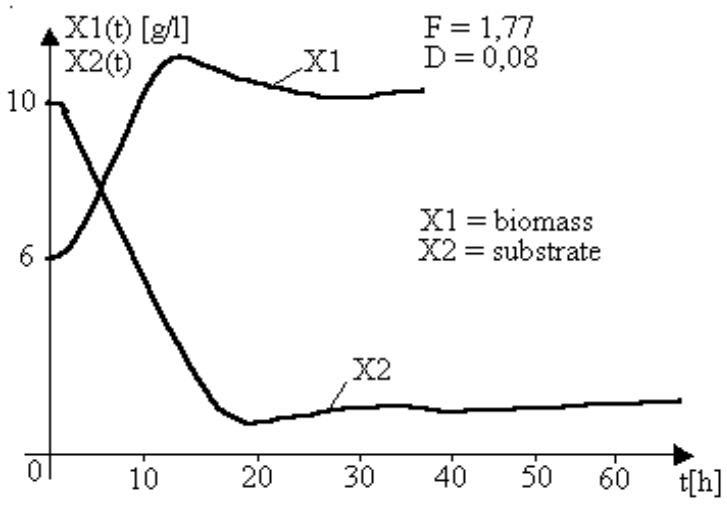

Figure 2

CONCLUSIONS

General mathematical model used in the simulation of the fermentation process is a structural-functional one, resulted from methodological-classical approach based on the material and thermal balance equations.

For the studied application the next assumptions regarding the process were admitted:
- the existence of a culture medium with a single specie of microorganisms X(t);
- the alimentation of the culture medium is done with a single substrate having the concentration S(t);
- the biomass growing rate μ(t) was admitted as depending on the alimentation substrate and on the biomass concentration X(t) existent at one moment in bioreactor.
- the alimentation rate with substrate had been considered constant.
- the utilization of a parameterization of the biomass growing rate μ(t), (Monod type), dependent only on alimentation substrate concentrations had proved inefficient in this case.
- the utilization of a parameterization of μ(t) and function of microorganism's concentration from the system, is considered more than necessary in the case when it is asked for higher performance indicators.
- for a strict control, in optimal conductions of the biological processes case, the approach to the biological state of the microorganisms (ex: the utilization of the age distribution of the microorganisms in the dynamics evaluation of the biotechnological processes) can be very useful.

In conclusion, because of the complexity and variety of the biological phenomena and their profound nonlinearities, the generalization of some methods become practically impossible, and every biological process, while a detailed approach, may constitute a different case.

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