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 progress on global plan and also on national plan too. A distinct interest can be remarked from the direction of control and optimization of fermentation processes with numerical calculator help. A determinative role in that way it has the construction of the model, the identification of the process, the estimation of the parameters and the analysis of the model.

The fermentation processes had some specific features, among will mention:

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

The important 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. MATHEMATICS MODELS OF THE FERMENTATION PROCESSES.

Fermentation represents the growing process of the microorganisms by different cultures for biosynthesise products. The growing of the microorganisms is watched from the determination of the cellular mass, cellular density or microorganisms 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 is necessary to take care of other quantities too, like: phosphorus, nitrogen, and temperature that depend by specific conditions of the studied process.

The models basic structure of a fermentation device in continuous flux with concentrates parameters can be introduced in that form:

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

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

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

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

where:

X is the active biomass concentration;
S is the organic substrate concentration;
C is the dissolved oxygen concentration;
P is 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 utilization speed that is in relation with the growing and maintenance of the respiration.

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

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 had 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. Those had lead us to use 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

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

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 identification of the parameters was realised by simulation using the method of the sensibility functions.

Was used the following optimisation criterion:

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

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

Had been derived the criterion function reported 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 $i = 1, 2, \ldots, 5$.

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 $s\mu_{pj} = \frac{\partial \mu}{\partial pj}$

$i,j=1, 2, \ldots, 5$.

The model parameters were determined minimizing the criterion function.

In stationary conditions will obtain the equations:

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

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

Resolving the system formed with equations (15) and (16) will obtain two stationary regimes:

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

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

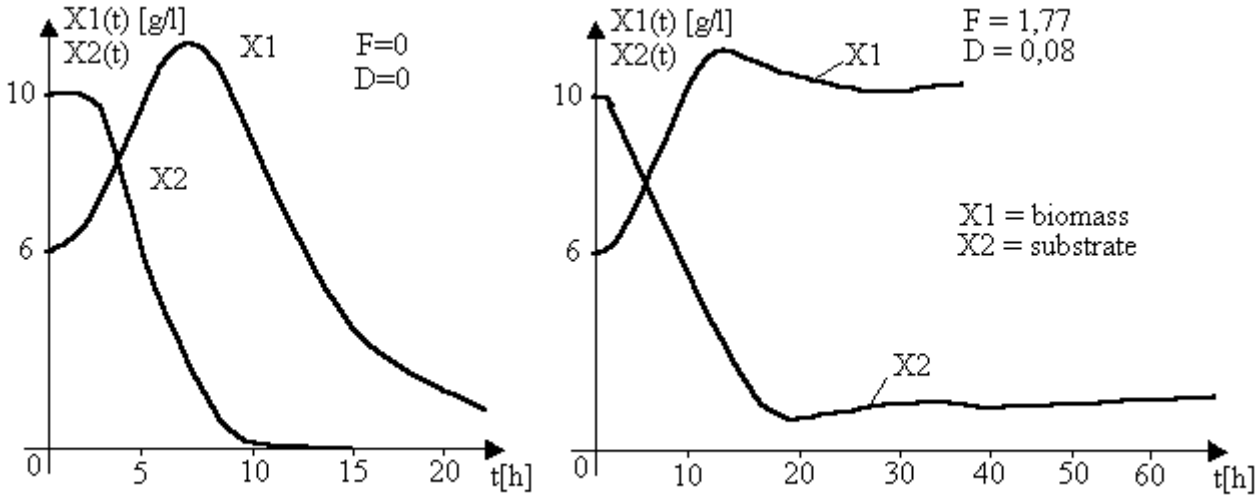
The system (17) constitutes the real and physical realisable solution of the process. For numerical simulation were considered the identification values of the parameters: $p_1 = 0,212$; $p_2 = 1,428$; $p_3 = 0,087$; $p_4 = 0,123$; $p_5 = 1,521$ and like initials values $X_{10} = 6$g/l; $X_{20} = 10$g/l.

The calculator simulation results for the case of the discontinuous process are represents in fig.1a, and for the case of the continuous flow process in table 1 and fig.1b.

Analysing the obtained results comparing with measured dates we can say that the presented model describe precisely enough the studied fermentation process.

Table 1. The calculator simulation results for the case of the continuous flow.

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



a b

Figure 1. The calculator simulation results for the case of the discontinuous process (a), and for the case of the continuous flow process (b).

CONCLUSIONS

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

For the studied application were admitted the next assumptions regarding the process:

- the existence of a culture medium with single specie of microorganisms X(t);
- the alimentation of the culture medium is done with single substrate having the concentration S(t);
- the biomass growing rate μ(t) was admitted like depending at the alimentation substrate and at the biomass concentration X(t) existent in 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), depended only by alimentation substrate concentrations had proved inefficient in the studied process 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, can be very useful the approaching that watched the biological state of the microorganisms (ex: the utilization of the age distribution of the microorganisms in the dynamics evaluation of the biotechnological processes).

In conclusion , because of the complexity and variety of the biological phenomena's and profound unliniarities of these, the generalization of some studying methods become practical impossible on large aria, and every biological process , in a detailed approaching, may constituting a different case.

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