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Mathematical modelling of the hydrodynamic structure of flows in the apparatus for cultivating chlorella: Parametric identification of the mathematical model

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Abstract. This article discusses the mathematical modeling of the hydrodynamic structure of flows in the apparatus for cultivating chlorella and the parametric identification of the mathematical model. Since in the considered reactor there is rather active longitudinal and radial mixing, the diffusion model is still more acceptable. However, such a model is described by partial differential equations and is associated with certain difficulties associated with determining the coefficients of radial and longitudinal diffusion. Therefore, when describing such phenomena, it makes sense to resort to the cell model. The mathematical description of the hydrodynamic structure of flows in the form of a cell model consists of a system of linear differential equations of the first order. On the basis of the obtained kinematic equations and the control of the hydrodynamic structure of flows in the reactor, a generalized mathematical model of the microalgae cultivation process is being drawn up. The model of the process under consideration obtained by analytical methods is a system of equations describing various aspects of the research object, taking into accounts the kinetic parameters and real hydrodynamic regimes. These specific values of the coefficients can be used to solve various engineering problems.

1. Introduction

When compiling a mathematical model for the cultivation of chlorella, it is necessary to take into account the change in the concentration of substance C in time t and along the length of the cultivator, taking into account the real hydrodynamic structure of the flows.

The system of equations (1) describes the process of cultivation of microalgae, which is carried out in a periodic mode. When the set value X is reached, the process is transferred to a continuous mode in order to increase the productivity of cultivators and stable use of crops and nutrients [1].

$$\begin{cases} \dfrac{dx}{dt} = \mu x; \\ \dfrac{dS_{P_i}^{i}}{dt} = d_{\varepsilon}\mu x; \\ \dfrac{dS_{m_i}^{i}}{dt} = m_{\varepsilon} x; \\ \mu = \mu_m \dfrac{S_i}{K_{S_i}} exp\left[\dfrac{(pH-\varphi_1)^2}{{\delta_1}^2} - \dfrac{(T-\varphi_2)^2}{{\delta_2}^2} - \dfrac{(C-\varphi_3)^2}{{\delta_3}^2}\right]; \\ \dfrac{ds}{dt} = (\alpha_1 \mu + m_i)x \end{cases} \qquad (1)$$

Known typical models of ideal mixing, ideal displacement, combined - cell, diffusion models with a certain degree of accuracy can be used to formalize the hydrodynamic structure of flows in various cultivators interacting in terms of design.

The hydrodynamic structure of streams in cultivators is usually the closest to the typical model of ideal mixing. But since the process under consideration takes place in tubular cultivators, where l> d (l is the length, d is the diameter of the apparatus), then in the first approximation when l / d≥10 it is advisable to use the model of ideal displacement [2]. In accordance with this model, piston flow without stirring is applied along the flow with a uniform distribution of the substance in the direction perpendicular to the flow.

Since in the considered reactor there is rather active longitudinal and radial mixing, the diffusion model is still more acceptable. However, such a model is described by partial differential equations and is associated with certain difficulties associated with determining the coefficients of radial and longitudinal diffusion. Therefore, when describing such phenomena, it makes sense to resort to the cell model.

2. Method

The mathematical description of the hydrodynamic structure of flows in the form of a cell model consists of a system of linear differential equations of the first order:

$$\frac{1}{m} * \frac{dS_i}{dt} = \frac{1}{\tau_n}(S_{i-1} - S_i),$$

where i = 1,2,3 ... m.

The physical essence of this model is that in each cell the flow under consideration is subjected to instantaneous radial mixing, and there is no mixing between individual cells (the process proceeds at a sufficiently high linear velocity). The number of assumed cells of ideal mixing m is a parameter characterizing the cell model. It is known that if m = 1, then the cell model goes over to the full mixing model n → ∞, to the ideal displacement model.

When using the cell model to describe the hydrodynamics of real flows, it is important to choose the correct number of cells, since it reflects the degree of mixing in the apparatus. Therefore, its role in the egg model is similar to that of the Peclet criterion in the diffusion model. [2]

Practical calculations show that it makes no sense to take m too large, since the cell model with m> 10 cells reproduces the properties of the ideal displacement model with sufficient approximation.

When determining the number of cells in a number of cases, one can use the formal analogy between the Peclet number and the value. It turns out that there is a relationship between these parameters, which, with sufficient accuracy for practical calculations, is expressed by the following relationship:

$$m = \frac{W_\alpha}{2b_\alpha} = \frac{2P_\alpha}{2},$$

where W_α is the average linear flow rate,
α - linear coordinates of the system,
b_α - longitudinal mixing coefficient,
P_α - Peclet diffusion test.

This dependence can be used to determine m and apply in research instead of the diffusion cell model, which is much simpler. Based on formula (2), experimental data can be used to determine the number m of the cell model. The value of the Peclet criterion can be determined from the data on the distribution of the residence time of particles in the flow:

$$P_\alpha = \frac{2}{\sigma^2};\ \sigma^2 = \frac{\Delta t\sum_{i=1}^{n}\tau_i Cu_i}{t^2\Delta t\sum_{i=1}^{n}Cu_i}, \tag{2}$$

C is the concentration of the substance (%);
t - time, min;
τ is the average residence time of particles in the apparatus;
Δt is the integration step.

To determine the cells in the cell model, we carried out experiments on a cultivator with a capacity of 10 m^3. The conditions of the experiment corresponded to the requirements of the technological regulations. The volumetric consumption of nutrients was V = 1.4 m3 / h.

Ammonia water was used as an indicator in recording the experimental curves. The analysis of the hydrodynamic structure of the flows was carried out by the impulse method, according to which a impulse disturbance was given in the concentration of ammonia water in an amount of 120 liters. The average residence time of particles in the apparatus was determined according to the generally accepted formula:

$$t = \frac{\Delta t\sum_{i=1}^{n}tCu_i}{\Delta t\sum_{i=1}^{n}Cu_i} \tag{3}$$

Calculations using this equation yielded the following results:
topt = 75 min
σ = 0.2.

Hence it follows that m = 4.8. We take the value of the number of ideal mixing cells equal to 5.

The impulse response (C - curve) for the cell model has the form

$$C_{\kappa p}(t) = \frac{1}{(m-1)!} * \left(\frac{mt}{t}\right)^{m-1} * \frac{m}{t}e^{-\frac{mt}{t}} \tag{4}$$

Theoretically - the curve (solid line) and experimental (dashed line) for the cell model (m = 5) are shown in Figure 1.

The divergence of the curves at the beginning and at the end of the process, from our point of view, is explained by the presence of stagnant and (or) other zones, which in their volume occupy a significant place with the main object of the cultivator.

3. Results and Discussions

Thus, based on the obtained kinematic equations (3) and control of the hydrodynamic structure of flows in the reactor (4), we compose the following generalized mathematical model of the microalgae cultivation process:

$$\begin{cases} \dfrac{dx_i}{dt} = \dfrac{V}{V_i}(x_{i-1} - x_i) + \mu_i x_i \\ \dfrac{dSp_{ij}}{dt} = \dfrac{V}{V_i}\left(Sp_{i-1,j} - Sp_{i,j}\right) - \alpha_i\mu_i x_i \\ \dfrac{dSm_{ij}}{dt} = \dfrac{V}{V_i}\left(Sm_{i-1,j} - Sm_{i,j}\right) - \mu_i x_i \\ \mu_i = \mu_m\dfrac{S_{ij}}{Ks_i + S_{ij}}\exp\left[-\dfrac{(ph-\varphi_1)^2}{\sigma_1^2} - \dfrac{(T-\varphi_2)^2}{\sigma_2^2} - \dfrac{(l-\varphi_3)^2}{\sigma_3^2}\right] \\ \dfrac{dS_{ij}}{dt} = \dfrac{V}{V_i}\left(S_{i-1,j} - S_{ij}\right) - (\alpha\mu_i + m)x_i \end{cases} \tag{5}$$

The next task is to determine the values of the coefficients included in equation (5).

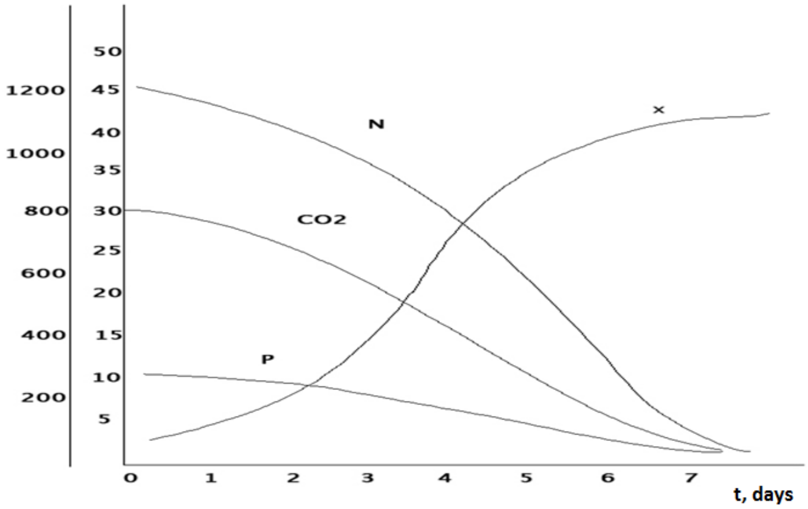

Figure 1. Changes in concentration of N, CO_2, P and X over time.1

The model of the process under consideration obtained by analytical methods is a system of equations describing various aspects of the research object, taking into accounts the kinetic parameters and real hydrodynamic regimes. These specific values of the coefficients can be used to solve various engineering problems. Determining the kinetic constants and model parameters that best reflect the experimental data is a very laborious and complex task. This is usually achieved by parametric identification methods [2].

The problem of parametric identification is to experimentally determine the characteristics of an object. The estimation of the parameters of the object is carried out within the framework of a mathematical model of a certain class. At the same time, the differences between the data obtained on a real object and on the corresponding mathematical model should be as minimal as possible. A detailed discussion of parametric identification methods, including the input and analysis of convergence conditions, can be found in [3].

In any case, any parametric identification method must yield parameter estimates that are unbiased, i.e. $E\{Q(N)\}= Q_0$ (6)

for finite Ne and are consistent in the mean sense, i.e.

$$\lim_{N_э\to\infty} E\{\hat{Q}(N_э)\} = \Theta_0 \quad (7)$$

$$\lim_{N_э\to\infty} E\{\hat{Q}/[\hat{Q}(N_э) - \hat{Q}_0\} = 0 \quad (8)$$

These methods are acceptable when the object is described by stable difference equations, as well as when the following conditions are met.

- the order of the object and the amount of delay must be known;
- changes in the input signal X (t) = X (t) –X0 are made without errors and the steady-state value of the input X0 is known;
- the input signal does not exceed the specified reaction order.

Moreover, the matrix

$$\mathrm{H} = \{\mathrm{h}_{ij} = y^n(\mathrm{i}-\mathrm{j})\}, \ \ \mathrm{i,j} = 1,2,\dots,\mathrm{m} \quad (9)$$

detH> 0.2 is positive definite and, in addition, there are limits

$$X_0 = \lim_{N_э\to\infty} \sum_{t=0}^{n-1} x(t); U, \quad (10)$$

$$\varphi(\tau) = \lim_{N_э\to\infty} \sum_{\tau=0}^{N_э-1} x(t) * (x(t)+\tau); \quad (11)$$

where τ is the shift time.

The output signal y (t) = y (t) –y0, as a rule, can be affected by disturbances. The steady-state value of y0 is considered known and is equal to the value of x0 multiplied by a static coefficient of the form

$$y_0 = y^* x_0 + E(t) \quad (12)$$

Equation error E (t) is not corrected with data items y (t). This means that these values are not statically known.

We will use these circumstances and conditions of identification and try to determine the necessary values of the coefficients included in equation (5).

Assuming that a solution to equation (5) exists and that measurements at the object of study are always feasible (with some error), we can assume that the quantities y (t) and x (t) depend on the measurement accuracy, the input noise and the correct choice the observed state vector.

To avoid a situation where small errors in experimental data can lead to large errors in determining the constants, an assessment of the correctness of the identification problem is required. In addition, the question of the sufficiency of experimental data arising in the study of competing models is important. These essential aspects are considered in works [2, 4, 5, 6].

During the cultivation of microorganisms, a lot of perturbations of a character are superimposed on the deterministic kinetic dependences, which explains the emerging need for periodic or constant adjustment of the model coefficients. The idea of adjusting the parameters of the model, the process of cultivation of microalgae was considered in [7], and in the most general form of the formulation of this problem was implemented in [8].

The problem of estimating constants is associated with a reliable choice of a method that provides the required accuracy and fast convergence of the search. At present, a fairly large number of methods for evaluating kinetic constants have been developed [2]. Among them, the most widespread are the least squares method, the maximum likelihood method and the method of estimates based on Bayes' theorem.

However, it should be noted that when evaluating kinetic constants, biochemical and microbiological reactions, a graphical method is still often used, which is inferior in accuracy to analytical ones and is difficult to formalize on a computer [7].

The coefficients α, m, β, γ included in the initial equations can be determined by the grapho-analytical method. We will use the following relations:

$$\frac{S(0)-S(t)}{\int_0^t x(t)dt} = \alpha\frac{x(t)-x(0)}{\int_0^t x(t)dt}, (13)$$

$$\frac{P(t)-P(0)}{\int_0^t x(t)dt} = \beta\frac{x(t)-x(0)}{\int_0^t x(t)dt} + \gamma, (14)$$

in the given ratios (13) and (14), the quantities *S (0), S (t), x (o), x (t), P (0), P (t)* represent the instantaneous values of the concentration of the substrate S, microorganisms x, products of metabolism P at time moments *0 and t,* value$\int_0^t x(t)dt$ is numerically equal to the area bounded above by the cell growth curve in the time interval from 0 to t.

Based on relations (13) and (14), it is necessary to carry out experiments using the method of graphic interpretation and, on this basis, construct graphs and then calculate the values of γ, m, β. In [7], the results of just such a determination of the values of these coefficients are presented.

Experience has shown that this method of conjugation with certain difficulties, especially for specialists who do not have sufficient experience in experimental research of technological processes. Only after numerous experiments and control calculations can one be sure of the correctness of the obtained coefficient values. Therefore, in order to overcome these difficulties, speed up calculations and obtain more accurate and reliable results, we used methods of approximate differentiation.

The biocatalytic process is described in general form by the equation;

$$y=f(c)$$

The f (c) values, as a rule, at the initial stage are the result of experiments. The obtained experimental data are plotted on a graph, where the abscissa is C, and the ordinate is t. The concentration of the substrate - S can act as C. culture - X or the concentration of any other substances of interest to us. For this purpose, experiments were performed, the results of which are shown in Figure 2.

As the concentration of the substrate (nutrients) changes within wide limits and has a direct connection with other biocatalytic processes and phenomena, it is more convenient and more accurate to determine the values of the coefficients of interest to us precisely through this parameter. The concentration - S of the substrate (concentration of nutrients) can also be determined more accurately and faster by experimental methods.

Whatever process is described by the function y = f (C) under consideration, the derivative Y 'from a physical point of view can be interpreted as the speed with which this process proceeds [9].

To find the derivatives of S '(X) on the interval [t_0, t], approximately replace the function with the Newton interpolation polynomial constructed for the required t_0, t_1,…, tn_0.

Then *S '(t)* for three points takes the following form:

$$S'(t) = \frac{1}{h}[\Delta S_0 + \frac{2q-1}{2}\Delta^2 S_0 + \frac{3q^2-6q+2}{6}\Delta^3 S_0] \ (15)$$

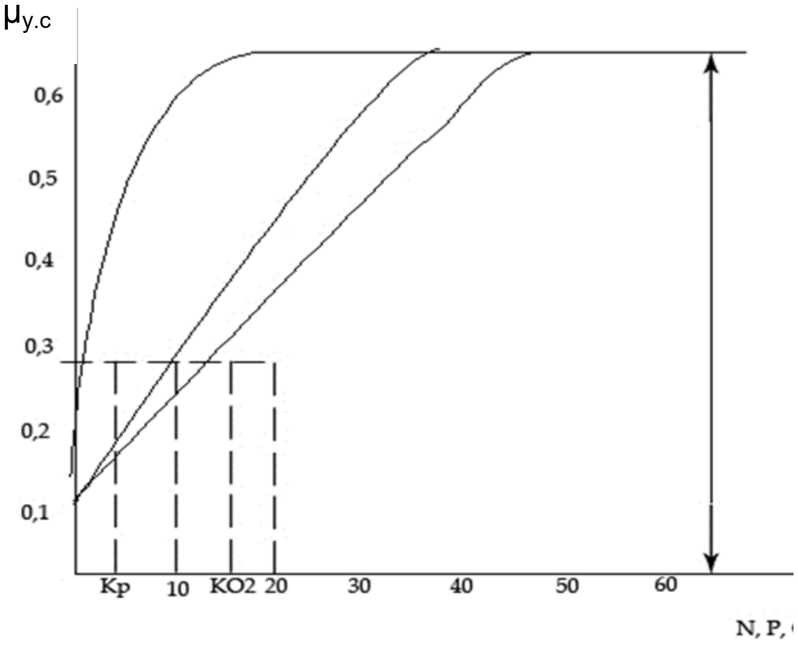

Figure 2. Dependence of the specific growth rate of chlorella on the concentration of nutrients P, N, CO_2

Where, $q = \frac{t_{i-1}-t_i}{h}$ is the number of steps required to reach point t from point t_0 and $h = t_{i+1} - t_i (t = 0,1,2,\dots,n)$.

Here, $\Delta S_0, \Delta^2 S_0 \, u \, \Delta^3 S_0$ is determined by the finite difference method. As a result, we get three algebraic equations with three unknowns in the following form:

$$\begin{cases} -S^{'}(t_0) = [\alpha\mu(t_0) + m + \beta\gamma(t_0)]X_0; \\ -S^{'}(t_1) = [\alpha\mu(t_1) + m + \beta\gamma(t_1)]X_1 \ (16) \\ -S^{'}(t_2) = [\alpha\mu(t_2) + m + \beta\gamma(t_2)]X_2 \end{cases}$$

Here the values $S^{'}(t_0), S^{'}(t_1), S^{'}(t_2)$ known: they are determined from the results of experiments; α, m, β unknown coefficients.

To solve the system of equations, we apply the method of successive elimination of unknowns (Poisson's method). As a result, we obtain

α^{N}=1,5; m^{N}=0,06; β^{N}=0,06;
α^{P}=1,3; m^{P}=0,05; β^{PP}=0,05;
α^{CO2}=1,1; m^{CO2}=0,02; m^{CO2}=0,02;

Analysis of the data obtained shows that the value of the coefficient β is always small. This indicates the fact that during the cultivation of microalgae chlorella, secondary products are practically not formed.

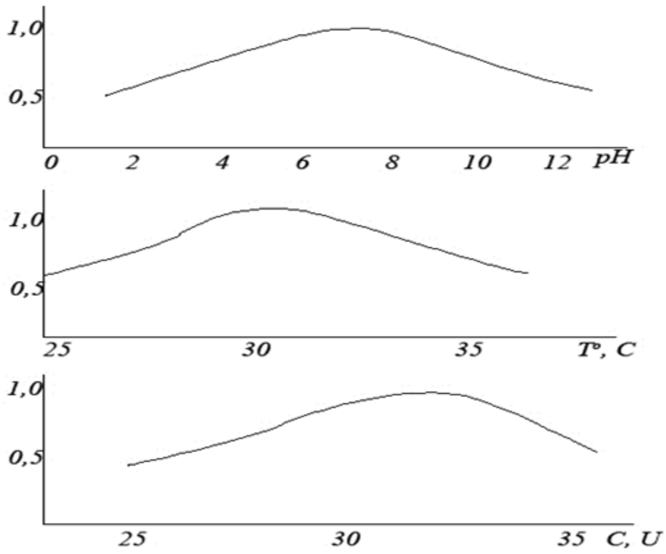

Figure 3. Dependences of μ on pH, T, C: α-μ on pH; β-μ from T; β-μ from C

This assumption is confirmed by the results of the analysis of the course of the investigated technological process. Thus, in further work with (16), we can take $\beta = 0$, which greatly simplifies the system of equations. The K_N^s value is determined from the dependence of the reaction rate on the substrate concentration. The specific rate of the enzymatic transformation of the substrate into biomass V_{yg} (Figure 3) is calculated by the formula

$$V_{yg} = \frac{S_0 - S}{t_i - t_1} * \frac{1}{x}\gamma \quad (17)$$

In production conditions, other nutrients (substrates) are also used, but they do not significantly affect the speed of the process. Therefore, in further calculations we will take into account only such significant factors as N, P, CO2. From the data in Fig. 3 the K_s values for N, P and CO_2 are determined. The values found in this way are as follows:

K_p =2; K_{CO2}=12; K_N = 17

The experimental dependences of μ on pH, T, C are shown in Figure 3.

4. Conclusions

As a result of processing the experimental data by the method of moments, the values of μ and δ were obtained. For μ, depending on pH, we have: Y1 = 6.7; δ = 6.2; for T: Yr = 29.8; for C: Y3 = 26.5.

Thus, having solved the problem of parametric identification of the proposed model, one can actually begin to study on a computer the results of modeling the process of chlorella cultivation.

References

[1] Rakhmanov Sh 2019 *Irrigation and Melioratio*n **2019** 132-135.
[2] Bondar AG 1973 Mathematical modeling of chemical technological processes, Higher School, Kiev.
[3] Romanovskiy OM, Stepanova NV, Chernyavskiy DS 1978 Mathematical biophysics, Science, Moscow.
[4] Kiryanenko VS 1973 Problems of automation of microbiological experiment, Guided microbial synthesis, Zinatne, Riga, pp 5-24.
[5] Muzaffarov AM, Taubaev TT 1974 Chlorella, Fan, Tashkent.
[6] Muzaffarov AM 1972 Cultivation of algae and higher aquatic plants in Uzbekistan, Fan, Tashkent.
[7] Akhmetov KA, Ismailov MA 1986 Mathematical modeling and control of technological processes of biochemical production, Fan, Tashkent.
[8] Smolyakov YuM, Yuriev AG 1977 *Fermentation and Alcohol Industry* **7** 22-24.
[9] Rakhmanov ShR 1993 *Sat. Problems of Cybernetics* **149** 117-121.