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Mathematical modeling of the extraction process of target components from yeast biomass

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A generalized mathematical model of the process of extraction of target components from yeast biomass (carbohydrates, lipids and ribonucleic acids)has been developed on the basis of experimental studies. It is substantiated that the theoretical provisions are satisfactorily consistent with the experimental results of the research. The obtained model allows to describe with sufficient accuracy the kinetics of extraction of carbohydrates, lipids and ribonucleic acids from yeast biomass, to determine the yield of the extract and to predict the optimal time of extraction in order to optimize and intensify the process, especially at the stage of designing extraction apparatus.

Keywords: *mathematical modeling; extraction; yeast; ribonucleic acids; bioactive compounds.*

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1. Introduction

Currently, mathematical modeling is the main research method in all fields of science and practice and a scientifically based method of evaluating the characteristics of complex systems. Mathematical modeling and forecasting of chemical technology processes, that are characterized by the complexity of modeling objects and are variable in space and time, are especially relevant [1–4]. The method of mathematical modeling is widely used during the design of equipment [5, 6], the study of various technological processes [7, 8] and the establishment of technological parameters for their execution [1], the optimization of compositions' formulations [9] and the prediction of the characteristics and properties of finished products [10]. While studying complex technological processes, apparatus, properties or physical phenomena, it is a challenge to take into account all the factors: certain factors are the most important, and some of them can be neglected. The traditional way of solving such problems, based on conducting real experiments, commonly leads to significant time, material and energy costs [11, 12]. One of the main methods for solving this problem is the application of mathematical modeling [13–16], that allows to replace real objects with mathematical models with adequate representation of the most important regularities of the studied systems and phenomena. Experiment planning methods allow obtaining mathematical models of the investigated process in the most economical and effective way in the realized range of changes in many factors affecting the process.

Prediction of experimental results using mathematical modeling is especially relevant and important during the study of diffusion and extraction processes, which are widely used in the field of biotechnology, food production and agriculture [17–20].

2. Problem statement

Extraction is the removal of one or more substances from solutions or solids using solvents. At the same time, a transition of substances from a liquid phase to another liquid phase takes place. The extraction process differs from other removal and separation methods by such advantages as high efficiency and selectivity; low operating temperatures; profitability of extracting valuable components and harmful impurities from diluted solutions; the possibility of a beneficial combination with rectification, chemical precipitation; relative simplicity of hardware design; the possibility of full automatization of

the process [18]. The extraction process is one of the most effective methods of separating mixtures and exudating products in their pure form [18, 21]. In particular, extraction is used to remove lactic acid and antibiotics from enzymatic solutions, lipid and protein components from cell mass, components from plant raw materials (olive seeds, sugar beets, fruits) [22–25]. In practice, in technological production, the task of hardware and technological design of these processes often arises, resulting in the need for their modeling. Obtainment of valuable products based on biomass processing is one of the promising areas of microbiological, pharmaceutical, chemical and other industries. Yeast is a rich source of proteins, antioxidants, vitamins and other bioactive compounds [26–28].

One of the important products that can be obtained from yeast biomass is ribonucleic acids (RNA) [29], which are widely used as raw materials for the production of ribonucleotides, nucleotides, and various pharmacological drugs. Therefore, obtaining highly purified RNA in combination with biological activity is, at present, an actual challenge [30, 31], in particular using the extraction method without utilizing chemical reagents; this provides an opportunity to use fodder yeast more fully and comprehensively [32].

Nowadays, theoretical foundations of this process are not sufficiently studied. There is no comprehensive process model that takes into account the membrane properties of the yeast biomass shell and the possibility of controlled extraction. Intensification of technological processes of extraction is also an urgent task. Intensification consists in acceleration and full use of interacting substances. Aimung to evaluate the influence of various factors on individual stages of the extraction process and their overall effect, it is necessary to express these dependencies using mathematical models allowing to calculate the parameters of the process and find optimal modes of its implementation. The implementation of the intensified process of target components extraction from yeast biomass is associated with obtaining calculation equations that allow determining the duration of extraction and rational parameters of the extraction mode. Modeling the extraction process enables its study at the design stage with certain technological parameters.

Thus, the purpose of this paper was to develop an adequate mathematical model of the extraction process of target components from yeast biomass.

3. Description of the modeling object

Extraction of target components from yeast biomass (carbohydrates, lipids, RNA, etc.), from a kinetic point of view, is complex. The extraction rate of the target components is relatively high in the initial period of time, and then slows down significantly. Thus, the entire mass of extracted components found in a particle of yeast biomass can be divided into two parts. The first part is removed relatively easily due to the absence of barriers that prevent the penetration of both the solvent and the extracted substance through them. The second part is more difficult to pass into the solution, because it is more isolated.

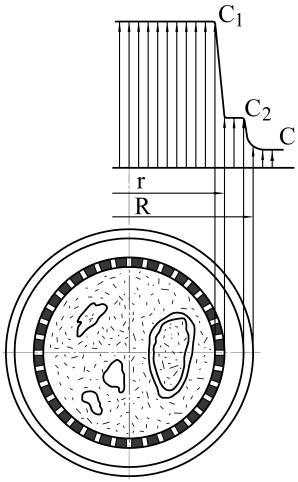

Fig. 1. A model of a spherical cell of yeast biomass.

The diffusion coefficients calculated on the basis of conventional theoretical solutions are of the order of $10^{-15} - 10^{-16}\,\mathrm{m}^2/\mathrm{sec}$, being $7 - 5$ orders lower than the free diffusion coefficients of carbohydrates. Low diffusion coefficients can be explained by the effect of certain factors – the structure of the yeast biomass cell, its nature, agglomeration of biomass cells during drying, etc. A yeast cell is separated from the environment by a mechanically strong cell wall up to $(16 - 25) \cdot 10^{-12}\,\mathrm{m}$. The cell wall sometimes reaches 1/7 of the cell diameter and makes up from 15% to 30% of its dry weight [33].

During the study of the distribution of carbohydrates and lipids in various components of the yeast cell, it was established that on the surface of the cell there are carbohydrates from 18% to 30%, lipids from 6% to 21%; in the cell membrane – carbohydrates – $9 \div 60\%$, lipids – $30 \div 80$ %.

Research results show that the cell diaphragm divides the cell into two different volumes (strongly isolated internal and external) each with different extraction rates. To create a mathematical model of the extraction process of target components from yeast biomass, let us assume that during the interaction of the solvent with the biomass, a solution with a significant concentration limited in the cell is formed. Later, the dissolved substance diffuses into the surrounding fluid through the porous partition of the cell membrane. It is the cell diaphragm that creates the main resistance to the transfer of matter. The cell diaphragm divides the cell into two different volumes – internal and external, and release will occur at different rates [34, 35]. On this factor the mathematical model of the release of target components from yeast biomass is built.

A spherical cell model is adopted for the mathematical description of the process, simplifying the problem (Figure 1).

4. Results and discussion

During the interaction of biomass with a solvent, a solution with a concentration C_1 is formed inside the cell, then the dissolved substance spreads into the medium that is in direct contact with the cell wall, with C_2 concentration. From this medium, the solute diffuses into the main part of the solution with a concentration C. It can be seen from Figure 3 that the main resistance to the extraction of target components is created by the cell wall (similar to any membrane process), corresponding to the highest concentration gradient.

The change in the amount of substance inside the cell over time can be determined by the equation:

$$-\frac{4}{3}\pi R^3 \frac{dC_1}{d\tau} = 4\pi R^2 K_1 (C_1 - C_2),$$

and after the transformation it has the following form:

$$-\frac{dC_1}{d\tau} = \frac{3K_1}{R}(C_1 - C_2). \tag{1}$$

The change in the substance content in the inner part of the cell, within $R - r$, is determined from the equation:

$$-\frac{4}{3}\pi \left(R^3 - r^3\right) \frac{dC_1}{d\tau} = K_2 C_2\, 4\pi R^2 - (C_1 - C_2)\, K_1\, 4\pi r^2. \tag{2}$$

The right-hand side of equation (2) takes into account the inflow of the substance to outer part of the cell and the decrease of the substance outside its borders. This equation after transformation will be as:

$$-\left(1 - \frac{r^3}{R^3}\right) \frac{dC_1}{d\tau} = \frac{3K_2}{R} C_2 - \frac{3K_1}{r} \frac{r^3}{R^3} (C_1 - C_2).$$

After introducing the following notation: $\frac{r^3}{R^3} = \alpha$, one can get:

$$-(1 - \alpha) \frac{dC_1}{d\tau} = \frac{3K_2}{R} C_2 - \alpha \frac{3K_1}{r} (C_1 - C_2).$$

Let's use the following notations:

$$\tau' = \frac{3K_1 t}{r}, \quad \frac{\alpha}{(1-\alpha)} = \delta, \quad \beta = \frac{K_2}{K_1} \frac{r}{R} \frac{1}{(1-\alpha)}, \quad \delta + \beta + 1 = 2m, \quad K_1 = \frac{D_1}{\delta}, \quad K_2 = \frac{D_2}{\delta},$$

where D_1 and D_2 are diffusion coefficients of target components.

Taking into account the accepted notations, equations (1) and (2) after some transformations are as follows:

$$-\frac{dC_1}{d\tau'} = C_1 - C_2, \tag{3}$$

$$-\frac{dC_2}{d\tau'} = \beta C_2 - \delta (C_1 - C_2), \tag{4}$$

$$-\frac{dC_2}{d\tau'} = \beta C_2 + \delta \frac{dC_1}{d\tau}. \tag{5}$$

After solving equations (3)–(5) by the operational method, we get

$$\frac{C_1}{C_0} = \frac{P_1 - 2m}{P_1 - P_2} e^{-P_1\tau'} + \frac{P_2 - 2m}{P_1 - P_2} e^{-P_2\tau'}, \tag{6}$$

$$\frac{C_2}{C_0} = \frac{P_1 - 1 - \delta}{P_1 - P_2} e^{-P_1\tau'} + \frac{P_2 - 1 - \delta}{P_1 - P_2} e^{-P_2\tau'}, \tag{7}$$

where $P_{1,2} = -m \pm \sqrt{m^2 - \beta}$, C_0 is initial concentration of the extracted component.

Let us denote the total content of the target components, corresponding to a certain τ by M, then

$$M = C_1 \frac{4}{3}\pi r^3 + C_2 \frac{4}{3}\pi \left(R^3 - r^3\right).$$

The initial content of the target components will be denoted as M_0, so

$$M_0 = C_0 \frac{4}{3}\pi R^3.$$

The ratio of the current content of the target components to their initial content in the cell can be represented as

$$\frac{M}{M_0} = (1 - \alpha)\frac{C_1\delta + C_2}{C_0}. \tag{8}$$

Taking into account equations (6) and (7), equation (8) takes the following form:

$$\frac{M}{M_0} = (1 - \alpha)\left(\frac{\delta\,(P_1 - 2m) + P_1 - 1 - \delta}{P_1 - P_2} e^{-P_1\tau} + \frac{\delta\,(P_2 - 2m) + P_2 - 1 - \delta}{P_1 - P_2} e^{-P_2\tau}\right). \tag{9}$$

Let us mark:

$$A = \frac{\delta\,(P_1 - 2m) + P_1 - 1 - \delta}{P_1 - P_2}, \quad P_1 = a,$$

$$B = \frac{\delta\,(P_2 - 2m) + P_2 - 1 - \delta}{P_1 - P_2}, \quad P_1 = b.$$

Then equation (9) is in its final form:

$$\frac{M}{M_0} = 1 - \frac{C}{C_{\max}} = A\,e^{-a\tau} + B\,e^{-b\tau}. \tag{10}$$

The isolation of coefficients A, B, a, b in equation (10) was carried out by the method of steepest descent when searching for the minimum of the quadratic form:

$$S = \sum_{i=l}^{n} \left[\left(\frac{M}{M_0}\right)_e - \left(\frac{M}{M_0}\right)_t\right]^2, \tag{11}$$

where $(M/M_0)_e$ is an experimental value of the relative content of the target components in the yeast biomass cell; $(M/M_0)_t$ is a theoretical value of the relative content of the target components in the biomass cell, calculated according to the equation (10).

From relation (11) it can be concluded that

$$S = F(A, a, b).$$

The minimum of the function S corresponds to the best mean square deviation of the sought parameters value in the Eq. (10). The steepest descent method was implemented with the coefficient values in Table 1.

Table 1.

#	Target component	A_{1-3}	a_{1-3}	B_{1-3}	b_{1-3}
1.	Carbohydrates	0.895	0.55	0.105	0.029
2.	Lipids	0.900	0.45	0.100	0.035
3.	RNA	0.889	0.059	0.113	0.00165

Figure 2 presents the curves of the extraction kinetics of carbohydrates, lipids, and ribonucleic acids, calculated according to equation (10), as well as experimental data. Figure 3 shows the correlation dependence of the obtained results.

The analysis of the given data shows that the theoretical provisions, on the basis of which the analytical function containing two exponents was obtained, are in satisfactory agreement with the experimental results.

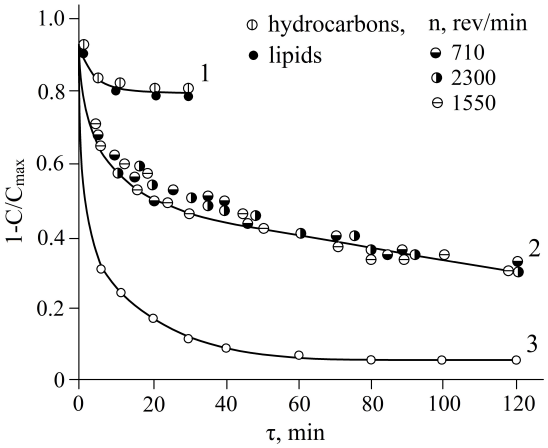

Fig. 2. Kinetics of release of carbohydrates, lipids and ribonucleic acids from yeast biomass (solid lines are values calculated according to the Eq. (10), dots are experimental values): 1 — release of carbohydrates and lipids from yeast biomass (an extractant is hexane); 2 — release of a mixture of carbohydrates and lipids from individual cells of yeast biomass at different rotation frequencies of the stirrer (an extractant is ethanol); 3 — release of RNA from yeast biomass (an extractant is water).

Experiments on the extraction of target components from yeast biomass were carried out on an installation consisting of an apparatus with a stirrer at a constant temperature according to the following method. A weight of biomass was loaded into the apparatus with a stirrer, after the extractant was poured inside at a certain constant temperature. Hexane, ethanol, and water were used as extractants. Samples were collected using a special sampler, than filtered and analyzed for the content of carbohydrates, lipids and RNA according to the appropriate methods [36–38] after certain time intervals. Figure 4 shows the results of the obtained experimental values of concentrations during the extraction of carbohydrates, lipids, and RNA from yeast biomass.

Based on the analysis of the data presented in Figures 2 and 4, it was established that the highest degree of extraction of carbohydrates and lipids is achieved from individual cells (curve 2). The additional resistance that occurs during the formation of cell agglomerates in the drying process is the reason for the relatively low level of extraction of the specified components from biomass particles. The high degree of RNA extraction is explained by the fact that water is used as an extractant in the extraction process, wherein biomass particles break up in water into individual cells and are destroyed at elevated temperatures.

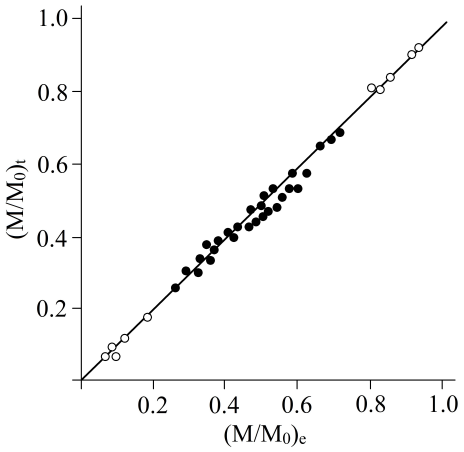

Fig. 3. Correlation dependence of experimental and theoretical results obtained during the extraction of target components from yeast biomass.

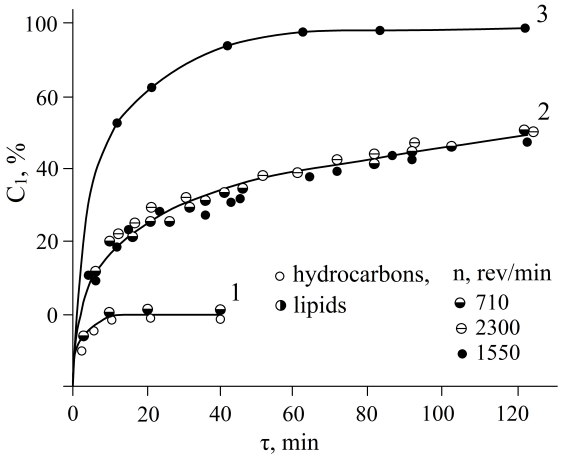

Fig. 4. Kinetics of release of carbohydrates, lipids and ribonucleic acids from yeast biomass: 1 — release of carbohydrates and lipids from yeast biomass; 2 — release of a mixture of carbohydrates and lipids from individual cells of yeast biomass at different rotation frequencies of the stirrer; 3 — release of RNA from yeast biomass (an extractant is water).

Thus, the Eq. (10) can be used to predict the extraction kinetics of target components from structures that are complex in terms of diffusion, such as yeast biomass particles.

5. Conclusions

A mathematical model for the extraction of target components from yeast biomass was developed. The adequacy of the developed model was examined and the possibility of its use for prediction of extraction kinetics of carbohydrates, lipids, RNA from biomass was presented.

It was established that theoretical provisions are in satisfactory agreement with the experimental study results. It was verified that the extraction process of carbohydrates and lipids is controlled by internal diffusion. The main resistance during diffusional release of target components is the cell wall and cell membranes.

A mathematical model enabling to predict the optimal time of extraction of target components from yeast biomass has been developed.

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Математичне моделювання процесу екстрагування цільових компонентів з біомаси дріжджів

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У даній роботі на основі експериментальних досліджень розроблено узагальнену математичну модель процесу екстракції цільових компонентів з біомаси дріжджів. Встановлено, що теоретичні положення задовільно узгоджуються з експериментальними результатами досліджень. Одержана модель дозволяє з достатньою точністю описати кінетику вилучення вуглеводів, ліпідів та РНК з біомаси дріжджів, визначати вихід екстракту та прогнозувати оптимальний час екстракції з метою оптимізації та інтенсифікації процесу, особливо на етапі проектування екстракційних апаратів.

Ключові слова: *математичне моделювання, екстракція, дріжджі, рибонуклеїнові кислоти, біоактивні сполуки.*