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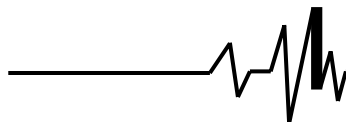
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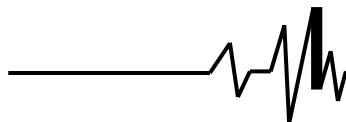
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**Vinnitsia National Agrarian
University****УДК 66.061.34****MODELLING OF OILY RAW
MATERIAL EXCRACTION
PROCESS**

This paper concentrates on approaches to mathematical modelling of oily raw material extraction process. «Evolution» of modeling hypothesis based on analysis of differential diffusion equation under the right boundary and initial conditions; on simplified model of Fick's equation and on material balance equation; on mass transfer model in adsorption pore volume; on model for the surface layer by analogy of Van der Waals equation; on Gibbs' model based on the abrupt change of phases due to the intermolecular forces; on the simplest Langmuir equation model; on lattice-based models of Guggenheim, Pryhozhyn, Everett, Ohm, Briukhovetskyi and others. The fact that we need to know a large number of micro - parameters makes these models difficult to use in practice.

Under normal extraction conditions, the flow, which comes out of solid phase, collides with the resistance of the diffusion boundary layer, which presents a tangible obstacle affecting the duration and quantity of special-purpose component extraction. As the boundary layer thickness depends on the hydrodynamics of the process, under the influence of the microwave field his obstacle is almost insensible, as the intense movement of liquid reduces its thickness. The main factor acting on the quantity of extracted substance is a pressure difference in capillaries and in the flow of extraction agent and mass transfer coefficient. The effect of pulse microwave input during the extraction transfers the process of diffusion from the external environment to internal, because internal pressure diffusion dominates in this process, but not the convective diffusion with the influence of external agent.

Keywords: *mathematical model, extraction process, oily raw material, material balance equation, process of diffusion, extraction agent.*



During oily seed extraction under the influence of the microwave field, following processes occur: firstly, the special - purpose component transfers from capillary - porous structure to liquid. Secondly, diffusion processes combined with mixing of environments through turbulent fluctuation. Thirdly, pressure diffusion processes appearing because of electromagnetic field influence. Due to the influence of field energy influence, which concentrates in the liquid phase of the capillary seed, vapor bubbles are formed. This causes the emergence of the pressure gradient and oil from the capillary under the oscillating mode is periodically pushed out into the stream. Intensification factor of extraction process, including the most common – increase in temperature, does not considerably improve special-purpose component extraction in the capillary.

The microwave field impact on the extraction process also requires long studies. When exposed to pulsed field under oscillating mode with three massive flows, another flow of extracted substances occurs. Pressure diffusion, caused by increased pressure leads to the formation of cavitation bubbles, which intensify the process and extract the hardly accessible component into the overall flow of the narrow - diameter capillary. That is why the main purpose of this article is a theoretical study and development of mathematical description of extraction process, based on a mathematical model simplification.

PURPOSE OF RESEARCH. The aim of our theoretical study was to develop a mathematical description of the extraction process based on a simplified mathematical model. If we concentrate on the transfer from micro - parameters to macro - parameters, given the effect of temperature on the extraction process, we will obtain a semi - empirical model of the process describing the technological process, and coefficients of the models will have their specific physical meaning. This mathematical model is useful for the examination of the extraction process. Numerical methods with the electronic computers are used to find solutions based on this model (system MATHCAD, MATLAB, etc.).

Material and methods. Mathematical models of extraction process, described in the studies of Akselrud G.A. [1, 4, 5, 6], are based on the analysis of differential diffusion equation under appropriate boundary and initial conditions.

$$\frac{dC}{dt} = D \left(\frac{d^2C}{dx^2} + \frac{d^2C}{dy^2} + \frac{d^2C}{dz^2} \right). \quad (1)$$

Under boundary conditions:

$$D \left(\frac{dC}{dn} \right)_n = K(C_{II} - C). \quad (2)$$

Material balance equation:

$$(C_0 - C) = C_p - C.$$

Initial conditions $\tau = 0, C = 0$

$$\left(\frac{dC}{dx} \right)_{x=0} = \left(\frac{dC}{dy} \right)_{y=0} = \left(\frac{dC}{dz} \right)_{z=0} = 0, \quad (3)$$

where C – current concentration of special-purpose substances in solid phase; τ – time; dx, dy, dz – change of coordinates on time; D – internal diffusion coefficient; K – mass transfer coefficient; C_{II} – concentration on the particle surface, C_0 – initial concentration of the substance in a solid phase; C_p – concentration of the substance in the solute.

Fedorchuk - Moroz V.I. [1, 7] mentioned in her study the simplified extraction kinetics model of special - purpose components of oily seed of the family Amaranthaceae. This model is based on Fich's equation (4) and on material balance equation (5):

$$\frac{dM}{d\tau} = -D_{cm} \cdot F \cdot \frac{dC}{dx}, \quad (4)$$

$$M = C_1 \cdot W = V \cdot (C_{II} - C), \quad (5)$$

where M – mass of the substance subject to extraction; D_{cm} – coefficient of compressed diffusion; F – surface area of a sphere, m^2 ; $(dC/dx)_{r=R}$ – concentration gradient; x – linear dimension; C_1 – concentration of the substance in the basic mass of solute; W – amount of solvent; V – volume of the sphere.

Common solution of equations (4) and (5) with boundary conditions $C_{I\tau=0} = C_{II}$ is the following equation:

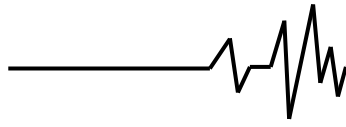
$$1 - \frac{C_1}{C_K} = \exp \left(- \frac{3 \cdot K \cdot \tau}{R} \cdot \left(\frac{C_{II}}{C_{II} - C_K} \right) \right), \quad (6)$$

where C_k – final concentration of the solute; R – radius of particle; K – coefficient of extraction; $K = D_{cm} / \delta$, δ – thickness of the glume.

The paper defines kinetic constants for the objects mentioned above. According to equation in semi logarithmical coordinates,

$-\ln \left(1 - \frac{C_1}{C_K} \right) = f(\tau)$ we got the possibility to define the constant K , based on the equation $tg \alpha = \frac{3 \cdot K}{R} \cdot \left(\frac{C_n}{C_n - C_k} \right)$.

Variables $-\ln \left(1 - \frac{C_1}{C_K} \right) = f(\tau)$ for amaranth of size $d_c = (0,25 \text{ mm})$ at different temperatures, are calculated on the basis on equation 6. They were also compared with the experimental data.



More accurate math model which takes into account the special-purpose component distribution in the seed and in its cells is elaborated [7] on the basis of seed chipping.

System of equations constitutes the basis for this mode:

$$\left\{ \begin{aligned} &-\frac{4}{3} \cdot \pi \cdot R_i^3 \cdot \frac{dC_i}{d\tau} = \frac{D_{\Delta}}{\Delta} \cdot 4 \cdot \pi \cdot R_i^2 \cdot (C_i - C_{as}); \\ &C_a = \frac{1}{2} \cdot (C_{as} + C_{an}); \\ &\frac{4}{3} \cdot \pi \cdot (R_a^3 - R_i^3) \cdot \frac{dC_a}{dt} = 4 \cdot \pi \cdot R_i^2 \cdot D_{\Delta} \cdot \frac{C_i - C_{as}}{\Delta} = K \cdot C_{as} \cdot 4 \cdot \pi \cdot R_a^2; \quad (7) \\ &-D_a \left(\frac{dC_a}{d\tau} \right)_{\tau=R_a} = K \cdot C_{an}, \end{aligned} \right.$$

where C_i – oil concentration in the cells of the seed; R_i – radius of the sphere, which contains special-purpose component with concentration C_i ; D_{Δ} – coefficient of compressed diffusion thought the germ's zone; D_a – thickness of the zone, where germ is placed; C_{an} – concentration of the substance on the line of phase contact of the particle with the solvent; C_{as} – concentration on the line membranous wall – germ.

The first equation (7) contains a special-purpose components mass change in the seed on the left side and concentration gradient on the right side. The second equation (7) defines the average value of the oil concentration outside the seed. The third equation (7) on the left side presents mass content outside the cells. On the right side of this equation, we take into account the increase in the special-purpose component in a solvent.

The mass transfer model in adsorbing pore volume in the study of Vasylenko V.V. [1, 8] deserves further attention.

The process of oil extracting from the porous parts of the original oily raw material with the pores half-filled with oil, represented as a pore diffusion process in the cellular body. Vasylenko V.V. found that the velocity of diffusion in macro-cellular is much greater than the speed of diffusion in micro-cellular and therefore it is not a limiting stage, Vasylenko V.V. presented the mathematical kinetics model of pre - extraction of oily raw material combining it with the impregnation kinetics by following equation:

$$K = \int_0^{\tau} K_0(\theta) \cdot \frac{d}{d\theta} \left(\frac{M(\tau - \theta)}{M_0} \right) d\theta, \quad (8)$$

where $K_0 = \frac{c_0 - c}{c_0}$ – extraction rate; c_0

and c – concentration of extracted oil in the cellular of the solid phase; initial and current, kg/m^3 ; K i K_0

– extraction rate without impregnation and with impregnation; (θ) – adsorbed phase concentration.

In studies of Konstantinov E.N. [1, 9], taking into account the features of system, oily raw material is a solvent, we should mention, first of all, that before the extraction process, the oily raw material is processed, and undergoes mechanical stress, heat, frying, drying. As a result, we notice that there processes damage the intracellular structure and form pores that contain oil, and while extraction – solvent. This action leads to change of the forms of oil connection with the material.

Various researchers considered the issue of oil bonds of the oily raw material. It is believed that the oil is located in two states: firstly, oil is on the surface of particles - internal and external and, secondly, oil is located in undisturbed cells and pores. The basic amount of oil is capillary oil and only a small amount – surface oil [1, 10]. According to the classification of Rebinder, oil that is outside is called free, and oil, which is closed in the pores is bound [10]. A number of scientists hold the classification of Rebinder.

Due to the fact that the description of oil connection forms with the material is qualitative and not generalized by the theory, it can describe the balance in the system oily material – solvent. Konstantinov in his study developed a simple model that took into account only adsorption bonds [9]. Later this model was improved and the author called it «adsorption pore model». According to the «adsorption pore model», oil and solvent are located in the pores of the material where there is an interaction: oil and solvent molecules; the interaction of oil molecules with molecules of solvent; interaction between the solvent molecules and centers of absorption and centers of oil adsorption.

Development of lattice models is considered in studies of Guggenheim, Prihozyn, Everett, Ohm, Briukhovetsky and others [11, 12]. In this direction notable success was reached. Today there are two main approaches to the study of surface properties. In the first one, distribution limit is considered to be flat and takes into account the change in the normal direction to the surface of the solution components concentration for various molecules and solutions, monomers, polymers, binary and multicomponent mixtures. The second one consists in the direct modeling of heterogeneous parts of the system and in considering the related statistical sum [1, 2].

Within this area adsorption pore model has been developed [9]. Fluid model must be the basis for any model of liquid phase absorption. In this case, the model of capillary-porous system and the external fluid will be coordinated.



Regarding the kinetics of internal and external mass transfer during extraction of solid bodies and process of extraction modeling in the study of Konstantinov the following studies were conducted. According to the general theory of mass transfer, during interphase mass transfer of the substance occur at least two resistance transfers – in the case of extracting internal resistance (solid part) and external (liquid phase) mass transfer.

Mass transfer (or diffusion) is usually described by the diffusion equation. As a first approximation, the diffusion coefficient is constant. Because the process that takes place in a particle is transient, it is not complicated by other phenomena described by the diffusion equation:

$$\frac{\partial c}{\partial \tau} + \operatorname{div}(-D \operatorname{grad} c) = 0. \quad (9)$$

This raises the question of the boundary value problem with different initial and boundary conditions. A large number of works is dedicated to analysis and solution of these problems. During the analysis process, it was found that the diffusion coefficient is not constant. It was proposed to determine the variable D of experimental with the help of interval iterative method.

It can be noted that during the initial period the value «grad» tends to infinity near the division border and therefore the material flow is high. At the same time, in the analytical solutions which we obtain after using of endless orthogonal series, all members of the series have a value, and the tangent of slope angle of the kinetic curve in the coordinates of concentration complex ($\ln \bar{c}$) – Fourier number (F_0) does not characterize the diffusion coefficient. Therefore, a different approach is used, according to which some form of analytical variable D of the concentration is adopted and, based on the equation of non-stationary diffusion according to experimental data, the coefficients of this dependence are searched as identification parameters. In variants that are more pragmatic, they are limited to replacement of solutions with the help of two members of the series. In a result, we have a satisfactory description of the experimental kinetic curves.

Approach that takes into account the physics of the process of the substance mass transfer in capillary - porous medium (which is the oily material) is much more physically reasonable. In this case, the movement of «free» substance in the pore environment and related by the force of interaction with the solid body is considered [13, 14]. Most clearly, the idea presented in studies [3, 15, 16, 17] focuses on the distribution of mixtures on molecular-implanted adsorbents (such as ion exchange resin). This process is related to the process of extracting as sorption with desorption.

Overall material balance for the liquid phase and adsorbent is as follows:

$$\frac{\partial c_\epsilon}{\partial \tau} + \frac{\partial c_\epsilon}{\partial z} - D_z \cdot \frac{\partial^2 c_\epsilon}{\partial z^2} = - \left(\frac{1 - \epsilon_\epsilon}{\epsilon_\epsilon} \right) \left(\frac{3}{R} \right) D_l \frac{\partial c_p}{\partial r} \quad r=R, \quad (10)$$

where ϵ_ϵ – difference of substance.

The equation takes into account the longitudinal (axial) mixing based on diffusion model of a longitudinal mixing ratio of the liquid phase, which has a concentration c_ϵ and also diffusion transfer in a particle with concentration – c_p .

Internal transient mass transfer in spherical wedge is described by the equation:

$$\epsilon_p \frac{\partial c_p}{\partial \tau} + \rho(1 - \epsilon_\epsilon) \frac{\partial q}{\partial t} = \epsilon_p D_l \left(\frac{\partial^2 c_p}{\partial r^2} + \frac{2}{r} \frac{\partial c_p}{\partial r} \right), \quad (11)$$

where ϵ_p – difference of solvent.

In this case, the change of amount of «free» substance (c_p) and of substance associated by adsorption forces (q) through «free» stuff substance diffusion (D_l) is considered.

In general, we can note that the diffusion coefficient in the solid particle is significantly lower than diffusion coefficient in the liquid phase.

This approach, which helps to describe mass transfer, in spite of its severity, may be used with caution for describing the process of plant raw material extracting. This is due to the irregular shape of the particles, to mesh-size distribution, which is broad enough, and to continuity of the process. The latest indicates that diffusion during extraction takes place most of the time in a regular mode. In this regard, scientists used in their works the method of splitting the total resistance of mass transfer from solid material to the liquid βh [9]. This approach requires an experiment on mass transfer kinetics for the purpose of evaluation of the approximate equations and direct use of the data received in the calculation of the extractor.

Currently extraction process modeling under the influence of microwave fields is described for the processes «coffee - water» [1, 19] and «oak - hydro alcoholic solution» [19]. Other sources [20 - 26], despite the diversity of research areas, do not present mathematical description of the extraction process.

The study of Piashko G. M. [18] presents the mechanism of combined mass transfer process of extractive substances from porous structure of coffee beans into solute. Distribution of concentrations «solid body - solvent» happens from the inside section through the outer area through capillaries in the near - boundary diffusion layer.

Results. Few assumptions were made for this solution:



1) the speed of the solution movement is constant throughout the cross section of the capillary;

2) soluble substance diffuses from the surface of the channel to the flow.

In this case, the diffusion equation is shown in cyclic coordinates on the current radius r [1, 18]:

$$w_0 \frac{\partial x}{\partial z} = D \frac{1}{r} \frac{\partial}{\partial r} \left[r \frac{\partial x}{\partial r} \right]. \quad (12)$$

Variable $D \left(\frac{\partial^2 x}{\partial z^2} \right)$, which characterizes diffusion through the channel is relatively low in comparison with convection component $w_0 \left(\frac{\partial x}{\partial z} \right)$.

Boundary conditions are as follows:

$x = x_p$, if $z = 0$ for all r ; $x = x_3$, if $r = 0,5d$ (d – the size of the extractable particle) for all z .

Application of Bessel functions of the first kind I_0 i I_1 leads to the equation:

$$\frac{x - x_p}{x_3 - x_p} = 1 - 2 \sum_{n=1}^{\infty} \frac{I_0(a_n r / 0,5d)}{I_1(a_n)} \exp\left(-\frac{D}{w_0 r^2} a_n^2 z\right), \quad (13)$$

The average concentration at the outlet of the channel at z , equal to its length, is calculated after integrating (13):

$$\frac{x_p'' - x_p'}{x_3 - x_p'} = 1 - 4 \sum_{n=1}^{\infty} \frac{1}{a_n} \exp\left(-\frac{Da_n^2 z}{w_0 0,25d^2}\right), \quad (14)$$

where a_n – value r for which $I_0(r)=0$.

For parabolic velocity profile in accordance with the Navier-Stokes equations:

$$w_{\max} \left[1 - \left(\frac{r}{0,5d} \right)^2 \right] \frac{\partial x}{\partial z} = D \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial x}{\partial r} \right). \quad (15)$$

Taking into account the limit concentration of the formula (15) equation is as follows:

$$\frac{x_p'' - x_p'}{x_3 - x_p'} = 1 - \sum_{n=1}^{\infty} a_n \exp - b_n \left(\frac{D}{w_{c.p} 0,25d^2} \right) z, \quad (16)$$

where $w_{c.p} = 0,5w_{\max}$ – average velocity flow rate; a_n i b_n – constants.

When considering the removal kinetics of spherical model porous bodies [15] the following simplification was prevented: they isolated on body

surface an area, for which the boundary layer thickness δ extractant is much shorter than the length of the selected area. The surface of rapeseed and soybean rape is presented as a plate, washed by thin laminar extractant layer.

Longitudinal velocity W , changed from 0 on the sphere surface to $w\delta$ on the outer sphere boundary. Diffusion equation, which establishes the distribution concentration in time τ at one point, convective concentrations change during the transition from point to point, depending on the velocity components and W_x, W_y are as follows:

$$\frac{\partial c}{\partial \tau} + w_x \frac{\partial c}{\partial x} + w_y \frac{\partial c}{\partial y} = D \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right). \quad (17)$$

The right side of equation (17) describes molecular diffusion.

They pursued the objective to determine the function $C(\tau, x, y)$ in the sphere δ , believing that the geometric dimensions of the highlighted areas significantly exceed the thickness δ . Using the method of two-dimensional complex Fourier transform with the infinite limits of integration in initial and boundary conditions

$$c \Big|_{x=\infty} = \frac{\partial c}{\partial x} \Big|_{x=\pm\infty} = 0, c \Big|_{y=\pm 0} = \frac{\partial c}{\partial y} \Big|_{y=\pm\infty} \quad (18)$$

they received the solution, believing that

the components of velocity W_y and W_x are given and do not depend on the coordinates, the diffusion process is not dependent on coordinates z . Assuming that the required function $C(\tau, x, y)$ satisfies the Dirichlet conditions on the interval $(-\infty, +\infty)$ on variables x, y and conditions in the area (18), we have:

$$c(\tau, x, y) \Big|_{\tau=0} = \exp[-(|x| + |y|)] \quad (19)$$

After determining the two-dimensional transform in the required function and after performing the double integrating, we replaced exponential expression by first term of its expansion in formal power series, given the symmetry of the problem, and found a solution of boundary problem



$$c(\tau, x, y) = \frac{1}{(1 - D\tau)^2} \left\{ \exp[(w_x + w_y)\tau - (|x| + |y|)] + D\tau \exp \frac{1}{\sqrt{D\tau}} [(w_x + w_y)\tau - (|x| + |y|)] - \right. \quad (20)$$

$$\left. \sqrt{D\tau} \left\{ \exp \left[\left(w_x + \frac{w_y}{\sqrt{D\tau}} \right) \tau - \left(|x| + \frac{|y|}{\sqrt{D\tau}} \right) \right] + \exp \left[\left(w_y + \frac{w_x}{\sqrt{D\tau}} \right) \tau - \left(|y| + \frac{|x|}{\sqrt{D\tau}} \right) \right] \right\} \right\}$$

Solution (19) also involved known diffusion coefficient D [18].

In [18] a model of diffusion from a point source into the flow was also considered. Under the proposed mechanism of mass transfer (Fig. 1) in addition to the solution (14), the pressure diffusion action is also provided.

When exposed to the electromagnetic field, pressure gradient within the open one-sided pore or capillary (R_{BD}) and in the flow of extractant (P_E) increases. Provided that $P_{BD} > P_E + P_K$, an emission is released into the fluid flow from the capillaries. Hydraulic resistance capillary P_K is also taken into account.

Diffusion flux of extractive components released into the extractant flow that moves in the direction Z with a constant rate W_0 . In this case, they solved the equation:

$$w_0 \left(\partial x / \partial z \right) = D \nabla^2 x, \quad (21)$$

with the following boundary conditions:

$$x|_{l=\infty} = 0; \quad \text{if } l \rightarrow \infty$$

$$4\pi l^2 D (\partial x / \partial r) = w_A, \quad \text{if } l \rightarrow 0.$$

$$l^2 = x^2 + y^2 + z^2, \quad (22)$$

where l – distance from the source; Z – distance downstream from the source; W_A – velocity with which extractive components are in flux.

Where the flow rate is constant (W_0), and the regime is stabilized, the solution (17) with boundary conditions (22) was as follows:

$$x = \frac{W_A}{4\pi D l} \exp \left[- \left(\frac{W_0}{lD} \right) \cdot (l - z)^2 \right]. \quad (23)$$

The problem of point source had practical importance in the analysis of concentration profile in the flow.

In the above models, we need to know a large number of micro - parameters, which make it difficult to use in practice. In the case of moving in this model (13) from micro - parameters to macro - parameters, taking into account the effect of temperature on the extraction process, we obtain a semi-empirical model of the process:

$$C = A - \frac{\alpha}{T} e^{-\gamma}, \quad (24)$$

where C – concentration of oil in the solution; A – the maximum concentration of oil in the solution at the given conditions of the experiment (solid phase particle size, the type of solvent, effect of microwave fields); α – coefficient characterizing the effect of temperature on the process of extraction; γ – coefficient characterizing the speed of the process at a given temperature; T – temperature process at any given time.

The mathematical model fairly well describes the process, and the coefficients A, α, γ have specific physical meaning. Thus, the mathematical model (24) should be used for research of extraction.

Let us develop a system of equations for the normal method of least squares (OLS) for the model (24). The objective function for (24) is as follows:

$$f(A, \alpha, \gamma, C_i, \tau_i) = \sum_{i=1}^n (C_i - C_{Pi})^2, \quad (25)$$

where C_i – experimental value of concentration in the solution;

C_{Pi} – the concentrations obtained in the modeling.

$$C_i = A - \frac{\alpha}{T} e^{-\gamma_i}, \quad (26)$$

The objective function for the equation (25) is as follows:

$$f(A, \alpha, \gamma, C_i, \tau_i) = \sum_{i=1}^n \left(C_i - \left(A - \frac{\alpha}{T} e^{-\gamma_i} \right) \right)^2. \quad (27)$$

Let us find the partial derivatives of the objective function (27) within the parameters A, α, γ .

$$\begin{cases} \frac{\partial f}{\partial A} = -2 \sum_{i=1}^n \left(C_i - A + \frac{\alpha}{T} e^{-\gamma_i} \right) \\ \frac{\partial f}{\partial \alpha} = 2 \sum_{i=1}^n \left(C_i - A + \frac{\alpha}{T} e^{-\gamma_i} \right) \frac{1}{T} e^{-\gamma_i} \\ \frac{\partial f}{\partial \gamma} = -2 \sum_{i=1}^n \left(C_i - A + \frac{\alpha}{T} e^{-\gamma_i} \right) \frac{\alpha \tau_i}{T} e^{-\gamma_i} \end{cases} \quad (28)$$

After equating the partial derivatives to zero, we have an equation as follows:



$$\begin{cases} \sum_{i=1}^n C_i - \sum_{i=1}^n A + \frac{\alpha}{T} \sum_{i=1}^n e^{-\gamma t_i} = 0 \\ \frac{1}{T} \sum_{i=1}^n C_i e^{-\gamma t_i} - \frac{A}{T} \sum_{i=1}^n e^{-\gamma t_i} + \frac{\alpha}{T^2} \sum_{i=1}^n e^{-\gamma t_i} = 0 \\ \frac{\alpha}{T} \sum_{i=1}^n C_i t_i e^{-\gamma t_i} - \frac{\alpha}{T} A \sum_{i=1}^n t_i e^{-\gamma t_i} + \frac{\alpha^2}{T^2} \sum_{i=1}^n t_i e^{-\gamma t_i} = 0 \end{cases} \quad (29)$$

After the elementary transformation of the system of equations (29), we get an equation as follows:

$$\begin{cases} \sum_{i=1}^n c_i - n \cdot A + \frac{\alpha}{T} \sum_{i=1}^n e^{-\gamma t_i} = 0 \\ \sum_{i=1}^n C_i e^{-\gamma t_i} - A \sum_{i=1}^n e^{-\gamma t_i} + \frac{\alpha}{T} \sum_{i=1}^n e^{-2\gamma t_i} = 0 \\ \sum_{i=1}^n C_i t_i e^{-\gamma t_i} - A \sum_{i=1}^n t_i e^{-\gamma t_i} + \frac{\alpha}{T} \sum_{i=1}^n t_i e^{-2\gamma t_i} = 0 \end{cases} \quad (30)$$

After organizing the system of equations (30), we obtain a system of normal equations of least squares method for nonlinear dependence:

$$\begin{cases} C = A - \frac{\alpha}{T} e^{-\gamma t} \\ \begin{cases} n \cdot T \cdot A - \alpha \sum_{i=1}^n e^{-\gamma t_i} = \sum_{i=1}^n C_i \\ T \cdot A \sum_{i=1}^n e^{-\gamma t_i} - T \sum_{i=1}^n C_i e^{-\gamma t_i} - \alpha \sum_{i=1}^n e^{-2\gamma t_i} = 0 \\ T \cdot A \sum_{i=1}^n t_i e^{-\gamma t_i} - T \sum_{i=1}^n C_i t_i e^{-\gamma t_i} - \alpha \sum_{i=1}^n t_i e^{-2\gamma t_i} = 0 \end{cases} \end{cases} \quad (31)$$

where, n – the number of paired values C_i , t_i ; C_i – concentration of oil in the solution (g/l); t_i – time extraction min.; T – temperature at any given time, K; and α, γ – unknown parameters.

The system of normal equations (31) of a mathematical model has no analytical solutions. Numerical methods with electronic machines are used (eg system Mathcad, Matlab, etc.) to find the solutions of systems of equations. Mathcad uses function “find” for the solution of nonlinear equation. This function is used in computing section Given. Given Block has the following structure (Fig. 1).

```

x:=1  y:=2  <- initial approximations Given
          x^2 + e^x + y = 30
x · y - y^2 = -5 <- simultaneous equations
          ( x1 ) := Find (x, y)
          ( y1 )
          ( x1 ) = ( 2,87141 ) <- system equation
          ( y1 ) = ( 4,09301 )
roots
x1^2 + e^x1 + y1 = 30  x1 · y1 - y1^2 = -5 <-
solution check
    
```

Fig. 1. Solving nonlinear equations with the help of Mathcad

In addition, Mathcad has a number of built-in functions for data analysis and regression that implement the method of least squares. Among them is a universal function “genfit”, which enables the least squares method to determine the unknown parameters for non-linear combinations of functions.

Genfit function has the format:

$$V = \text{genfit}(t, C, P, F), \quad (32)$$

where V – the vector of values of model parameters; t – a vector of values of the independent variable; C – vector of values of the dependent variable; P – vector of initial approximation; F – defined function in matrix form, which contains the function f (t) with unknown parameters A, α, γ and derivatives on these parameters (Fig. 2).

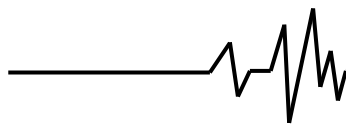
$$F(t, A, \alpha, \gamma) := \begin{pmatrix} A - \frac{\alpha}{T} \exp(-\gamma \cdot t) \\ \frac{1}{T} e^{-\gamma t} \\ -\frac{e^{-\gamma t}}{T} \\ \frac{\alpha \cdot t \cdot e^{-\gamma t}}{T} \end{pmatrix} \begin{matrix} \leftarrow \text{function} \\ \leftarrow \text{derivative at } A \\ \leftarrow \text{derivative at } \alpha \\ \leftarrow \text{derivative at } \gamma \end{matrix}$$

Fig. 2. Matrix form

So “genfit” function is useful for finding the unknown parameters of our model.

Data systems (Mathcad, Matlab) are widely used in the chemical and food industries to build mathematical models of processes.

Conclusions. In this paper, we propose a mathematical modeling solution of extraction process in a microwave irradiation in a form of semi-empirical model using numerical methods



with electronic machines (eg system Mathcad, Matlab, etc.).

The advantage of this model compared to the existing is the transition from micro - to macro - parameters, simplifying the proposed model, which makes it convenient to use in practice.

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МОДЕЛЮВАННЯ ПРОЦЕСУ ЕКСТРАГУВАННЯ ОЛІЄВІСНОЇ СИРОВИНИ

В статті розглядаються підходи до математичного моделювання процесу екстрагування олієвісної сировини. «Еволюція» гіпотез моделювання базувалась зокрема на аналізі диференційного рівняння дифузії за відповідних граничних і початкових умов; на спрощеній моделі рівняння Фіка та рівнянні матеріального балансу; на моделі масообміну в адсорбуючому поровому об'ємі; моделі для поверхневого шару за аналогом рівняння Ван-дер-Ваальса; моделі Гіббса, що базується на різкій зміні фаз завдяки дії міжмолекулярних сил; на найпростішій рельєфній моделі рівняння Ленгмюра; решітчастих моделей Гугенгейма, Пригожина, Еверетта, Ома, Брюховецького та ін. У зазначених моделях потрібно знати велику кількість мікропараметрів, що ускладнює їх використання на практиці.

При класичних умовах екстрагування потік, що виходить із твердої фази зустрічає на своєму шляху опір граничного дифузійного шару, який є відчутною перепорою, що позначається на тривалості та кількості вилучення цільового компоненту. Оскільки товщина граничного шару залежить від гідродинаміки процесу, то під дією

мікрохвильового поля його перепорою майже не відчутна, тому що інтенсивний рух рідини зменшує його товщину. Головним фактором, що діє на кількість вилученої речовини є різниця тиску в капілярі і в потоці екстрагента, а також коефіцієнт масовіддачі. Дія мікрохвильового імпульсного підводу при екстрагуванні переносить процес дифузії із зовнішнього середовища у внутрішнє, оскільки у процесі домінує не конвективна дифузія із впливом зовнішніх інтенсифікуючих факторів, а внутрішня бародифузія.

Ключові слова: математична модель, процес екстрагування, масляниста сировина, рівняння матеріального балансу.

МОДЕЛИРОВАНИЕ ПРОЦЕССА ЭКСТРАГИРОВАНИЯ МАСЛЯНИСТОГО СЫРЬЯ

В статье рассматриваются подходы к математическому моделированию процесса экстрагирования маслянистого сырья. «Эволюция» гипотез моделирование базировалось в частности на анализе дифференциального уравнения диффузии при соответствующих граничных и начальных условий; на упрощенной модели уравнения Фика и уравнение материального баланса; на модели массопереноса в адсорбированном поровом объеме; модели для поверхностного слоя аналогом уравнения Ван-дер-Ваальса; модели Гиббса, что основаны на резкой смене фаз благодаря действию межмолекулярных сил; на простейшей рельефной модели уравнения Ленгмюра; решетчатых моделей Гугенгейма, Пригожина, Эверетта, Ома, Брюховецкого и др. В указанных моделях нужно знать большое количество микропараметров, что затрудняет их использование на практике.

При классических условиях экстрагирования поток, выходящий из твердой фазы встречает на своем пути сопротивление предельного диффузионного слоя, который является ощутимой преградой, что сказывается на продолжительности и количества извлечения целевого компонента. Поскольку толщина граничного слоя зависит от гидродинамики процесса, то под действием микроволнового поля его преграда почти не ощутима, потому что интенсивное движение жидкости уменьшает его толщину. Главным фактором, который действует на количество изъятых вещества является разность давления в капилляре и в потоке экстрагента, а также коэффициент массопереноса. Действие микроволнового импульсного подвода при экстрагировании переносит процесс диффузии из внешней среды во внутреннюю, поскольку в процессе не



доминирует конвективная диффузия с влиянием внешних интенсифицирующих факторов, а внутренняя бародиффузия.

Ключевые слова: математическая модель, процесс экстрагирования, маслянистое сырье, уравнение материального баланса.

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