

# Mathematical modeling of the extraction process of oil-containing raw materials

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**Abstract.** A mathematical model for the extraction of oil-containing seeds in a one-dimensional formulation is considered. It is assumed that the seed petal as a modeling object has the form of a three-dimensional rectangular unlimited plate. The equation of nonstationary diffusion was chosen as a mathematical model and the third initial boundary condition was formed. Biot and Fourier diffusion criteria were determined. The problem is solved numerically using an implicit finite-difference scheme and the sweep method. The results of the theoretical study are compared with experimental data, which shows no more than 10% relative error.

## 1 Introduction

As is known [1-6], mass and heat and mass transfer processes are complex physico-chemical systems that have a dual determinant-stochastic nature with parameters varying in space and time. When these processes are carried out, momentum, energy and mass are transferred at each point of the phase and at the phase boundary, because the material and energy flows involved in the process are multiphase and multi-component. The components of these phases are characterized by random mutual influence on each other at the phase boundaries (productive orientation of the interphase boundary of moving media). Similarly, various systems are characterized by complex mutual influence of phases and constituent components, as a result of which it is impossible to study these systems from the perspective of the laws of conservation or transfer of classical deterministic matter.

To solve such a problem, it is necessary to use methods of system analysis of the object, mathematical modeling and finding the optimal solution. The basis of this strategy is the acceptance of processes as a complex mutually influencing hierarchical system, conducting a qualitative analysis of structures, assessing and determining parameters, their mutual influence, in particular, in the form of a mathematical description of the process [7-11].

Analysis of literary sources [1-6] shows that extraction processes require complex research, for example, mathematical modeling in close contact with the results of experimental studies of a single element of oil-containing raw materials.

Based on this, the purpose of this study is to construct a mathematical model of the extraction process in a solid element of raw material impregnated with an extractant.

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## 2 Theoretical basis

Extraction in a “solid-liquid” system, taking place in a stationary layer of solid material, is an unsteady process, because the concentration of the extracted component in the solid phase  $X$  changes both in space and time:

$$X = f(l, \tau), \quad (1)$$

where  $l$  is a geometric parameter;  $\tau$  – time, s.

The speed of the extraction process in this system depends on the following factors [2]: the magnitude of the driving force of the process; the speed of each stage of the process (transfer of a substance inside a solid particle, mass transfer from the surface of a particle to the extractant, swelling of particles, dissolution of the target component inside a particle); particle size and shape; the type of layer of particles that they form (mobile, stationary); mass ratio of extractant and solid particles; the nature of the relative movement of solid particles and extractant (countercurrent, forward flow); temperature and speed of phase movement. It is believed that the extracted component is contained in the pores of the solid in a dissolved state, then the extraction process is reduced to the extraction of the dissolved substance.

The molecular diffusion coefficient is a physical constant that characterizes the ability of a given substance to penetrate due to diffusion into a stationary medium. Depending on the process, what substance is extracted, the molecular diffusion coefficient differs from each other.

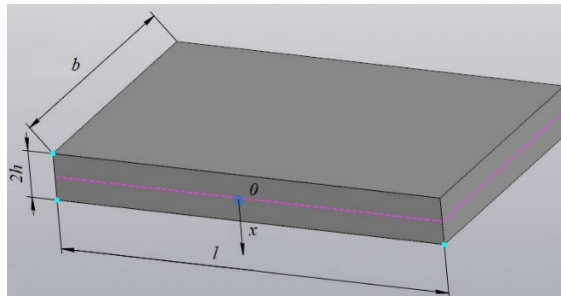
Intervals along the length of the apparatus (in time) must be large enough compared to the size of the extracted particles, but at the same time so small that the physical conditions of the process can be assumed to be constant within the interval, and the extraction line within the interval can be assumed to be straight.

Thus, the problem comes down to finding at the end of the interval the concentration field in a uniformly moving solid body of a certain shape and size under constant physical conditions, the linear nature of the change in concentration in the liquid, which is present in the solid body.

When mathematically modeling the extraction process, an abstract representation of the process is critical. To do this, it is necessary to introduce some restrictions and assumptions:

- the extraction process occurs at a constant temperature of the oil and extractant, the thermophysical and diffusion characteristics of the extraction object and extractant do not depend on temperature and time;
- since the geometric dimensions of the petal are  $l \gg 2h$  and  $b \gg 2h$ , then the field of concentrations of the petal in the raw material is assumed to be one-dimensional;
- the movement of the miscella from the center of the petal to its surface is carried out due to molecular diffusion, and the removal of the miscella from the surface of the petal into the liquid phase is due to convective diffusion;
- due to the symmetry of the cross section relative to the  $x$  axis, we take into consideration only one (right) half of the section of the petal with thickness  $h$ .

Thus, the object of modeling is a petal, which has the form of a three-dimensional rectangular plate with the following geometric dimensions: length,  $l$ , height  $b$  and thickness  $2h$  (Fig. 1).



**Fig. 1.** Simulation object.

Taking into account the accepted assumptions, we write the one-dimensional equation for non-stationary oil extraction from a swallow in Cartesian coordinates:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \tag{2}$$

where is  $D$  –the molecular diffusion coefficient.

To solve equation (2), we supplement it with the corresponding initial and boundary conditions.

We assume that the distribution of oil concentration in the cross section of the petal at the initial time (at time  $t=0$ ) is distributed equally:

$$C|_{t=0} = C_0, -h \leq x \leq h \tag{3}$$

Since half of the cross section of the petal is considered, we will take the symmetry condition as the first boundary condition:

$$\frac{\partial C}{\partial x} \Big|_{x=0} = 0, t > 0 \tag{4}$$

As the second boundary condition at ( $x = h$ , see Fig. 1), we take convective mass transfer, which is used in many sources [12, 13]

$$-D_m \frac{\partial C}{\partial x} \Big|_{x=h} = \beta(C_h - C_f), t > 0 \tag{5}$$

where is  $\beta$  –the mass transfer coefficient;  $D_m$  –mass conductivity coefficient;  $C_h$  –concentration miscella on the surface of a solid, (which is a function of time);  $C_f$  – concentration miscellas in the liquid phase.

The left side of equation (5) represents the diffusion flux density moving inside the petal towards the surface through mass conductivity. The right side of equation (5) represents the value of the density of the diffusion flux removed from the lobe to the liquid phase through convective diffusion.

Combining the above, we obtain the problem of a one-dimensional extraction process for extracting oil from a solid body - a petal, which has the form of a third initial-boundary value problem:

$$\begin{cases} \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} & 0 < x < h \\ C|_{t=0} = C_0 & 0 \leq x \leq h \\ -D_m \frac{\partial C}{\partial x} \Big|_{x=h} = \beta(C_h - C_f), t > 0 \\ \frac{\partial C}{\partial x} \Big|_{x=0} = 0, t > 0 \end{cases} \tag{6}$$

We will solve the problem in the full mathematical formulation (6) in dimensional variables by the finite difference method on a uniform grid. To do this, we divide the petal according to thickness  $h$  at  $N-1$  equal intervals, i.e. Let's construct a finite-difference grid [14]:

Replacing the differential operators in (1) with their finite-difference analogues using an implicit scheme, we obtain:

$$\frac{\partial C}{\partial t} = \frac{C_i^{n+1} - C_i^n}{\tau} \cdot \frac{\partial^2 C}{\partial x^2} = \frac{C_{i+1}^{n+1} - 2 \cdot C_i^{n+1} + C_{i-1}^{n+1}}{h^2}, i = \overline{2..N-1}, n = \overline{0..T} \quad (7)$$

Substituting these finite-difference analogues into (1) we obtain:

$$\frac{C_i^{n+1} - C_i^n}{\tau} = D \cdot \frac{C_{i+1}^{n+1} - 2 \cdot C_i^{n+1} + C_{i-1}^{n+1}}{h^2} \quad (8)$$

Carrying out some transformations in (8), we bring it to the following form:

$$A_i \cdot C_{i+1}^{n+1} - B_i \cdot C_i^{n+1} + D_i \cdot C_{i-1}^{n+1} = F_i \quad (9)$$

where the coefficients  $A_i, B_i, C_i$  have the following form:

$$A_i = \frac{D}{h^2}, B_i = \frac{2 \cdot D}{h^2} + \frac{1}{\tau}, D_i = \frac{D}{h^2}, F_i = -\frac{C_i^n}{\tau}$$

System (9) has a tri-diagonal structure, since we are solving a non-stationary problem, we will solve this system at each time step using the sweep method.

Using the sweep method, we look for a solution to system (9) in the form:

$$C_i^{n+1} = \alpha_i \cdot C_{i+1}^{n+1} + \beta_i \quad (10)$$

$$\text{At } i = 1, \text{ i.e. at } x = 0 \quad C_1^{n+1} = \alpha_1 \cdot C_2^{n+1} + \beta_1$$

Since when  $x = 0$  from (5)  $\left. \frac{\partial C}{\partial x} \right|_{x=0} = 0$ , whence  $C_1^{n+1} = C_2^{n+1}$

Then  $\alpha_1 = 1, \beta_1 = 0$ .

At internal points, the sweep coefficients  $\alpha_i, \beta_i$  are found by the formula:

$$\alpha_i = \frac{A_i}{B_i - D_i \alpha_{i-1}}, \quad \beta_i = \frac{D_i \beta_{i-1} - F_i}{B_i - D_i \alpha_{i-1}} \quad i = \overline{2..N-1}$$

At  $i = N, \text{ i.e. } x = l$

$$-D_m \left. \frac{\partial C}{\partial x} \right|_{x=h} = \beta(C_h - C_f) \quad (11)$$

Let us discretize this boundary condition with an error  $O(h^2)$ . Then for the derivative  $\frac{\partial C}{\partial x}$  we have

$$\left. \frac{\partial C}{\partial x} \right|_{x=h} = \frac{C_{N-2} - 4 \cdot C_{N-1} + 3 \cdot C_N}{2 \cdot \Delta x} \quad (12)$$

From (10) at  $i = N - 1$  and  $i = N - 1$  we have

$$C_{N-1} = \alpha_{N-1} \cdot C_N + \beta_{N-1}, C_{N-2} = \alpha_{N-2} \cdot C_{N-1} + \beta_{N-2}$$

Representing in the second expression  $C_{N-1}$  through the first expression we have:

$$C_{N-2} = \alpha_{N-2} \cdot C_{N-1} + \beta_{N-2} = \alpha_{N-2} \cdot (\alpha_{N-1} \cdot C_N + \beta_{N-1}) + \beta_{N-2}$$

Substituting expressions for  $C_{N-1}, C_{N-2}$  in (11) we obtain:

$$\left. \frac{\partial C}{\partial x} \right|_{x=h} = \frac{\alpha_{N-2} \cdot (\alpha_{N-1} \cdot C_N + \beta_{N-1}) + \beta_{N-2} - 4 \cdot (\alpha_{N-1} \cdot C_N + \beta_{N-1}) + 3 \cdot C_N}{2 \cdot \Delta x}$$

Inserting this expression for  $\left. \frac{\partial C}{\partial x} \right|_{x=h}$  into (11) we will have:

$$-D_m \left( \frac{\alpha_{N-2} \cdot (\alpha_{N-1} \cdot C_N + \beta_{N-1}) + \beta_{N-2} - 4 \cdot (\alpha_{N-1} \cdot C_N + \beta_{N-1}) + 3 \cdot C_N}{2 \cdot \Delta x} \right) = \beta(C_h - C_f)$$

Since  $C_f$  the concentration in the liquid phase is  $C_N$  from the last expression we have:

$$D_m \left( \frac{\alpha_{N-2} \cdot (\alpha_{N-1} \cdot C_N + \beta_{N-1}) + \beta_{N-2} - 4 \cdot (\alpha_{N-1} \cdot C_N + \beta_{N-1}) + 3 \cdot C_N}{2 \cdot \Delta x} \right) = \beta(C_N - C_h)$$

From the last expression after several transformations, we find  $C_N$ :

$$C_N = \frac{2 \cdot \Delta x \cdot \beta \cdot \frac{C_h}{D_m} - \alpha_{N-2} \cdot \beta_{N-1} - \beta_{N-2} + 4 \cdot \beta_{N-1}}{2 \cdot \Delta x \cdot \frac{\beta}{D_m} + \alpha_{N-2} \cdot \alpha_{N-1} - 4 \cdot \alpha_{N-1} + 3} \quad (13)$$

According to similarity theory, one can also obtain the Biot number from (11):

$$Bi = \frac{\beta \cdot h}{D_m}$$

The amount of extracted substance during extraction can be determined by the formula [15]

$$S = K \cdot F \cdot dC \cdot \tau \tag{14}$$

where is  $K$  –the total mass transfer coefficient, which for our case can be determined by the formula:

$$K = \frac{1}{\frac{h}{D} + \frac{S}{D_m}},$$

where is  $S$  –the thickness of the boundary layer,  $F$  –the contact surface of the media.

### 3 Results

To solve the initial boundary value problem (6), it is necessary to determine the values of the parameters characterizing the occurrence of mass transfer processes: diffusion coefficients, mass transfer and mass conductivity, and petal size.

According to sources [15,16], experimental and theoretical studies, the diffusion coefficient varies within  $10^{-7} \div 10^{-12} \text{ m}^2/\text{s}$ .

In [17], the value of the effective diffusion coefficient was  $1.44 \times 10^{-11} \div 1.73 \times 10^{-11} \text{ m}^2/\text{s}$ .

size also affects the optimality and duration of the extraction process; according to [18], the smaller the thickness, the maximum yield and speed of extraction. For example, according to [19], with a particle size of 0.3 mm in diameter, the yield of extractives was 98%. With this data in mind, we used the thickness in our calculations  $2h = 0.3 \text{ mm}$ .

Let us take the dimensions and properties of a grape seed petal according to the following values: length  $l = 5 \text{ mm}$ , width  $b = 4 \text{ mm}$ , density of the extractant  $\rho_{ekstr} = 471 \frac{\text{kg}}{\text{m}^3}$ , oil density  $\rho_{oil} = 930 \frac{\text{kg}}{\text{m}^3}$ , initial concentration of oil in the petal  $C_0 = 15\%$ .

In order to calculate the diffusion Fourier number, we also need the characteristic extraction time  $\tau$ . According to some data from the authors [13,15,20,21,22,23], the characteristic extraction time is one hour, i.e. approximately 3000 seconds. Then if we calculate the diffusion Fourier number ( $Fo_D > 0,25$ ), we get:

$$Fo_D = \frac{D \cdot \tau}{h^2} = \frac{1.5 \cdot 10^{-11} \cdot 3000}{0.0002^2} = 1.125$$

Thus, according to [24], at this value of the diffusion Fourier number, the regime of regular mass transfer is realized.

### 4 Discussion

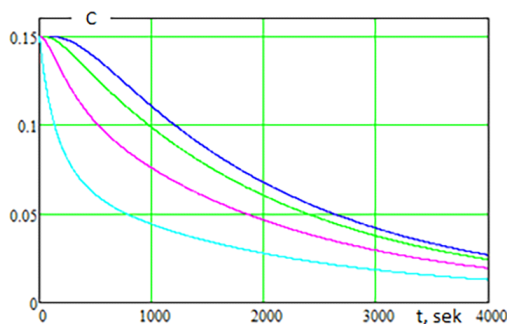
When calculating, we took the thickness of the petals  $h = 0.00015 \text{ m}$ , divide this distance into three segments in steps.  $\Delta x = 0.00005$ . We get four points along the axis  $x$ , the concentration value in the liquid layer  $C_h = 0.01$ .

Figure 2 shows the distribution of oil concentration in the petal by layer relative to the extraction time. As can be seen from Fig.2, the extraction of extractives from raw materials proceeded more slowly in the deep layer over time. According to the graph, in the outer layer the oil concentration decreases faster, i.e. here the oils in the outer layer are extracted relatively faster and the oil from the lower layer enters here. In general, in all quasi-layers, the oil concentration in the layers of the solid phase hyperbolically approaches the equilibrium state. The rate of oil extraction decreases over time, which is explained by a

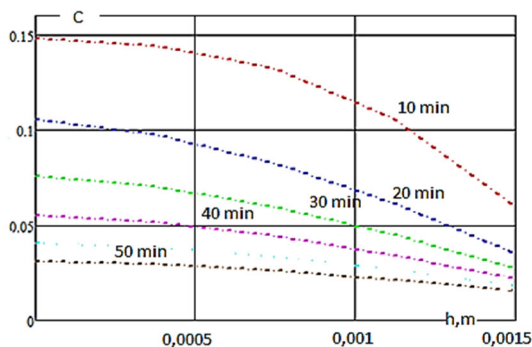
decrease in the concentration difference under the influence of which the oil passes from the petal to the extractant.

The study of the dependencies (Fig. 2) indicates that for maximum extraction of raw materials in the first stage, in which the oil concentration will be almost equalized over its entire cross-section, a time period of about 80 minutes is required.

Figure 3 shows the distribution of oil concentration over the thickness of the petal for different durations of the extraction process. As can be seen from Fig. 3, the concentration distribution at the beginning of the lobe gradually decreases due to the symmetric boundary condition. And at the end of the thickness there is the lowest point of concentration, which in the last layer the oil concentration decreases over time.

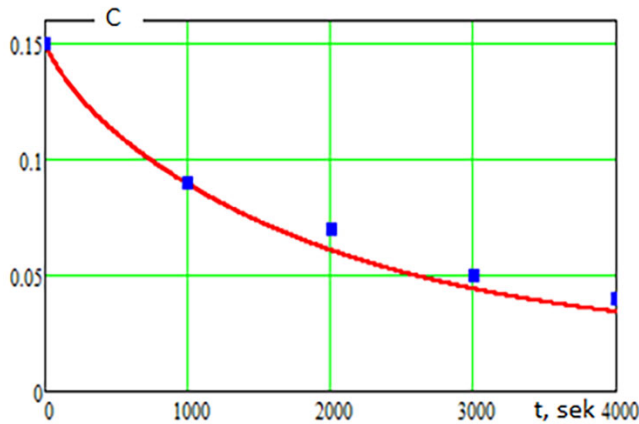


**Fig. 2.** Changes in concentration over time in different layers of the petal.



**Fig. 3.** Concentration distribution over the thickness of the petal for different durations of the extraction process.

Figure 4 shows the decrease in the average petal oil concentration over time. The model results are compared with experimental data [16,20,21]. The relative error is no more than 10%. Fig. 4 shows that there is a period of fast extraction, during which the process proceeds at the highest speed, and a second period of slow extraction, the speed of which is much lower. During the rapid extraction period, which lasts 1000 s, up to 60% of the substances contained in the raw material are extracted. This period is characterized by the extraction of substances with looser molecular structures and those located close to the surface of the raw material particles. The second period, the duration of which is 4000 s, is characterized by the extraction of substances contained deep in microcapillaries and inside undestroyed cells. During the second period, up to 25-30% of the oil remaining in the raw material is extracted.



**Fig. 4.** Change in grape seed petal oil concentration over extraction time. Experimental data points [16].

The amount of oil transferred from the petal to the outer layer is equal to the product of the mass transfer coefficient, the exchange surface and the difference in concentrations of the boundary and outer layers of the petal [13,15,24,25,26]:

$$M = k \cdot F \cdot (C_h - C_f)\tau \tag{15}$$

where  $k$  –the mass transfer coefficient, determined by the formula  $k = \frac{D \cdot \rho}{h}$ ,  $F$  –is the contact surface of the media.

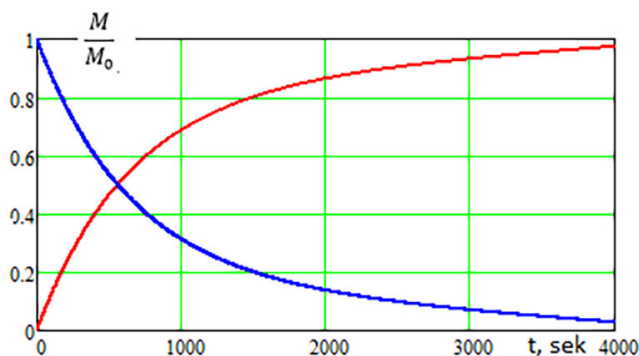
The density in the petal is determined depending on the concentration in the layer:

$$\rho = \rho_{ekstr}(1 - C) + \rho_{oil} \cdot C \tag{16}$$

Using the densities and petal sizes, the amount of oil present at the beginning of the extraction can be calculated. The oil content of grape seeds is approximately 15%. Then the amount of oil present in the raw material petal is equal to:

$$M_0 = \rho \cdot V \cdot 0,15 = 930 \cdot 0.0015 \cdot 0.008 \cdot 0.004 \cdot 0.15 = 4.8 \cdot 10^{-8}kg$$

Figure 5 shows the amount of oil extracted from the petal and the amount of oil remaining in the petal by extraction time.



**Fig. 5.** Change in oil concentration in solid and liquid phases over extraction time.

## 5 Conclusion

A mathematical model is formulated in the form of a diffusion equation with initial and boundary conditions corresponding to the extracted object for the extraction of oil-containing

raw materials. In this case, a grape seed petal in the form of a three-dimensional parallelepiped was chosen as the object of extraction. The problem is solved numerically using an implicit finite-difference scheme and the sweep method. Graphs of changes in concentration over time in layers of petal thickness and graphs of changes in oil concentration in the solid and liquid phase over extraction time were obtained. The results are compared with experimental data available in the literature, the average relative error of which does not exceed 10%. Thus, it can be assumed that the presented model is acceptable for engineering calculations of such processes.

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