

UDC 519.6+51-74::628.395

THREE-DIMENSIONAL MATHEMATICAL MODEL AND NUMERICAL SOLUTION ALGORITHM FOR MONITORING AND PREDICTING IN-SITU LEACHING PROCESSES IN POROUS MEDIUM

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The article analyzes the hydrodynamic processes associated with underground mining, in particular, the acid extraction of precious metals from ore deposits. In order to comprehensively study, monitor and predict the behavior of the object, a mathematical model (MM) based on the filtration-convection and diffusion processes characteristic of underground fluid filtration was developed. This model includes the influence of various hydrodynamic parameters, in particular, the filtration coefficient and average porosity, which are functions of the pressure level and process kinetics. Analysis of the problem statement shows that the change in pressure in the ore deposit resulting from the pouring and extraction of the solution directly affects the permeability and porosity coefficients of the layer. The experimental results showed that the change in hydrodynamic parameters was proportional to the change in pressure, with an exponential behavior observed under high pressure and a linear behavior under low pressure. It should be noted that in the process of in-situ leaching (ISL), a chemical reaction occurred as a result of the reagent's effect on the ore deposits, and the substance passed from one phase to another, as a result of which the hydrodynamic parameters of the pore medium (filtration and porosity coefficients) and pressure changes in the ore reservoir were observed.

Keywords: in-situ leaching, mathematical modeling, numerical algorithm, minerals, filtration and diffusion of liquids, kinetics of the process.

Citation: Ravshanov N., Usmonov L.S. 2025. Three-dimensional mathematical model and numerical solution algorithm for monitoring and predicting in-situ leaching processes in porous medium. *Problems of Computational and Applied Mathematics*. 6(70):26-47.

DOI: https://doi.org/10.71310/pcam.6_70.2025.03

1 Introduction

The discovery, development and effective use of valuable geological reinjection wells remains an important priority for all societies. The technological progress of our time requires the extraction and use of underground mineral reinjection wells. Therefore, the study of effective methodologies for the extraction of minerals is of great importance. The acceptance of ISL as an advanced technique is gaining momentum, therefore, the study, prediction and decision-making of the processes of underground filtration of liquids and gases requires the development of mathematical support that adequately reflects them and the conduct of computational experiments.

Scientific research has been conducted on the MM and study of ISL processes, and significant fundamental and practical results have been achieved.

[1] article was dedicated to the research, development and implementation of algorithms for solving MMs and filtration-diffusion problems, which were an important factor

for conducting comprehensive research and making management decisions in order to increase the efficiency of groundwater protection during the development of mineral deposits and acid treatment.

The main focus of [2] scientific research was on expanding the use of the ISL method and identifying effective strategies and tools for its use in the mineral deposits. In addition, monitoring the groundwater level in ISL areas is very important for hydrogeological studies. This monitoring helps to assess filtration processes, evaluate the performance of the technological solution, identify potential solution leaks, understand the hydraulic connections between productive geological structures, and determine the stability of the hydrodynamic regime in the area of interest.

In articles [3–5], MM and digital algorithm were given for liquid within the pore medium filtering three dimensional hydrodynamic process of ISL solution of problem Developed mathematical methods ore layers mastery parameters every side by side learning, injection and dig to take wells optimal placement choose, their stream speed assessment of groundwater pollution from injection wells protection to do provision factor to account to take possible gives. Because of the problem is described by a system of quasi-linear partial differential equations of the multidimensional parabolic type, obtaining an analytical solution is a difficult task. For digital integration task components according to division and the currents management from the methods used in case limited differences to the scheme based algorithm built. The proposed mathematical model can be used as a tool for analyzing and predicting the parameters of ore deposits and mineral extraction.

[6–8] mainly include the initial stage of leaching, a kinetically controlled process, a liquid-solid reaction in which the particle in question was transferred to the nucleus. Minerals in soluble acids are mainly dependent on the binding of the hydrogen ion to the anion, however, the overall dissolution rate was not related to the rate of this reaction, since such reactions were almost instantaneous.

Research [9–12] proposed to solve these problems by proposing a training data generation methodology adapted to the most reinjection well-intensive computational fluid dynamics problems encountered in the modeling of fluid flow in porous media. Traditional digital modeling from the methods entrance and suitable coming expected exit information included training information collection creation for used, in which well networks various to the forms separately attention given. Next actions taken data into neural networks suitable to format to convert directed. Data neural network in architecture applicable activation in functions in view caught information to the range adaptation for normalized. This initial processing to give phase of the neuron model created from the data effective to study provides, this and ISL processes exactly to predict makes it easier. Offer reaching of the equipment the advantage is on the ISL site currently active or expected technological modes based on hydrodynamic properties prophecy to do neural network for teaching for big, reliable information collection present from reaching consists of of this approach main meaning current in time in mining areas applicable expenses determination simulation aside past, future prophecy to do or in the layer the current hydrodynamic regime determination for in advance trained artificial intelligence technologies in use lies down. Thus, the innovative approach presented in these articles serves to overcome the computational barriers associated with traditional methods and optimize prediction, enabling faster and more efficient decision-making in reinjection well extraction operations.

In subsequent studies [13, 14], complex, closely interconnected technical systems (for example, sequential wells - pumping stations - reagent concentrators, etc.) were studied in the technological processes of mixing. It was shown that all of these subsystems are

interconnected and that a disruption in the technological regime of even one subsystem can lead to a complete shutdown of the entire work cycle. Therefore, the present in time many component systems work exit progressive to the methods big attention is being given, from them one is in-situ washing method. Compared to other methods, this method is considered the most economical and environmentally friendly approach, as its use does not lead to environmental degradation. This method is also widely used in the uranium mining industry, which is of great economic importance. The demand for energy from uranium, which is its main injection well, is constantly increasing. This observation emphasizes the importance of scientific research on effective methods of extraction of precious metals, in particular, the application of self-leaching process.

[15–18] scientific studies have investigated the processes of working with the ISL method in uranium deposits located in the Republic of Kazakhstan. Among the 15 active mining sites in Kazakhstan, SL offers a secure, dependable, and relatively cost-effective method for metal extraction. A significant challenge encountered during mining operations stems from the subterranean nature of the solution's interaction, as subsequent processes are concealed beneath the surface, thereby impeding effective decision-making [15]. Geological modeling involves delineating the ore body and characterizing the lithological and filtration properties of the formation [16]. Reference [12] underscores the application of mathematical modeling to develop a geological and technological model for uranium In-Situ Leaching (ISL), as well as its utility in addressing geotechnical and environmental challenges. Reference [13] offers comprehensive details on the implementation of a 3D reactive transport approach, utilizing the Hytec code, at an operational scale in Kazakhstan. The Hytec technology employs computational clusters to resolve mass transport issues, specifically to solve chemical equations for a broad spectrum of geochemical reactions, including aqueous complexation, oxidation-reduction, dissolution/precipitation, and sorption. Furthermore, this technology incorporates a hydrodynamic module that characterizes the filtration of solutions during ISL.

Current research [4, 5] works practical continuation as three dimensional mathematical model and numerical from the algorithm used in case, the matter time change according to solver programs complex and solution method offer is enough This issue the solution finding process filtration, diffusion and kinetic of processes together movement through to do is increased. of liquid movement to him impact doer volume or surface forces with is determined. Movable in liquid of substances to pass two completely other mechanisms through to the surface will come First, in liquid concentrations difference exists when, molecular diffusion occurs will be, secondly, in the liquid melted substance movement during the second one by pushing is taken. The combination of both processes is called convective diffusion of substances in a liquid. It should be emphasized that during the ISL process, the main hydrodynamic parameters of the research object change, firstly, as a result of changes in pressure in the porous environment, and secondly, as a result of the dissolution of material particles during acid treatment of the ore deposit.

Considering the above, this paper proposes a mathematical model to solve pressure and kinetic related problems in ore deposit.

2 Problem statement

Mathematical modeling of the ISL process for limited G in the field

$$G = \{(x, y, z, t), 0 < x < L_x, 0 < y < L_y, 0 < z < L_z, 0 < t \leq T\}.$$

useful concentration function of the component $C_2(x, y, z, t)$ to determine what for equation of the pressure field propagation elastic filtration process:

$$\begin{aligned} \beta m(x, y, z) h(x, y, z) \frac{\partial H(x, y, z, t)}{\partial t} = \frac{\partial}{\partial x} \left[k(x, y, z) h(x, y, z) \frac{\partial H(x, y, z, t)}{\partial x} \right] + \\ + \frac{\partial}{\partial y} \left[k(x, y, z) h(x, y, z) \frac{\partial H(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[k(x, y, z) h(x, y, z) \frac{\partial H(x, y, z, t)}{\partial z} \right] + \\ + F_1(x, y, z, t) - F_2(x, y, z, t), \quad [x, y, z] \in G, \end{aligned} \quad (1)$$

with initial condation:

$$H(x, y, z, t) = H^0(x, y, z), \quad t = 0, \quad (2)$$

and boundary conditions:

$$k(x, y, z) \frac{\partial H(x, y, z, t)}{\partial x} \Big|_{x=0} = -\alpha_1 \xi (H - H_0), \quad (3)$$

$$k(x, y, z) \frac{\partial H(x, y, z, t)}{\partial x} \Big|_{x=L_x} = \alpha_1 \xi (H - H_0), \quad (4)$$

$$k(x, y, z) \frac{\partial H(x, y, z, t)}{\partial y} \Big|_{y=0} = -\alpha_2 \xi (H - H_0), \quad (5)$$

$$k(x, y, z) \frac{\partial H(x, y, z, t)}{\partial y} \Big|_{y=L_y} = \alpha_2 \xi (H - H_0), \quad (6)$$

$$\frac{\partial H(x, y, z, t)}{\partial z} \Big|_{z=0} = 0, \quad (7)$$

$$k(x, y, z) \frac{\partial H(x, y, z, t)}{\partial z} \Big|_{z=L_z} = \alpha_3 \xi (H - H_0). \quad (8)$$

Here: $H(x, y, z, t)$ – pressure value, (m); $H^0(x, y, z)$ – initial pressure value, (m); m – porosity coefficient value; $k(x, y, z)$ – filter efficiency, (m/day); t – time (day); $h(x, y, z)$ – thickness of the ore horizon (m); β – coefficient of elastic capacity, (m²/kg); $\alpha_1, \alpha_2, \alpha_3$ – constants that take the values 0 or 1; L_x – length of medium by Ox axis (m); L_y – length of medium by Oy axis (m); L_z – length of medium by Oz axis (m); ξ – equation scaling factor (1/day);

$$F_1(x, y, z, t) = \sum_{i,j=1}^{N_1} q_{1,i}(t) \delta(x - x_{i,j}, y - y_{i,j}, z - z_{i,j}) - \text{power of the well};$$

$$F_2(x, y, z, t) = \sum_{i,j=1}^{N_2} q_{2,j}(t) \delta(x - x_{i,j}, y - y_{i,j}, z - z_{i,j}) - \text{power of the production well};$$

$q_{i,j}(t)$ – the power of the well; N_1, N_2 , respectively, the number of the production and injection wells; $\delta_{i,j} = \begin{cases} 1, & x = x_{i,j}, y = y_{i,j}, z = z_{i,j} \\ 0, & \text{other all condations} \end{cases}$ – Dirac is a delta function. (1)–(8)

using the finite difference method, we introduce the following dimensionless variables:

$$H^* = \frac{H}{H_0}, \quad x^* = \frac{x}{L_x}, \quad y^* = \frac{y}{L_y}, \quad z^* = \frac{z}{L_z}, \quad k^* = \frac{k}{k_0}, \quad h^* = \frac{h}{h_0}, \quad \tau = \frac{\varkappa_0 t}{L^2}, \quad \beta^* = \frac{\beta}{\beta_0},$$

$$q_{1,i}^* = \frac{q_{1,i} L^2}{\varkappa_0 H_0 h_0}, \quad F_1^* = \sum_i^{N_1} q_{1,i}^*(t) \delta(x - x_i, y - y_i, z - z_i), \quad H^{*0} = \frac{H^0}{H_0}, \quad \xi^* = \frac{\xi L}{\varkappa_0},$$

$$q_{2,j}^* = \frac{q_{2,j} L^2}{\varkappa_0 H_0 h_0}, \quad F_2^* = \sum_j^{N_1} q_{2,j}^*(t) \delta(x - x_j, y - y_j, z - z_j), \quad H^{*0} = \frac{H^0}{H_0}, \quad \xi^* = \frac{\xi L^*}{\varkappa_0}.$$

these substitutions into equations (1)-(8), we get:

$$\begin{aligned} & \beta^* m(x, y, z) h^*(x, y, z) \frac{\partial H^*(x, y, z, t)}{\partial t} = \\ & = \frac{\partial}{\partial x^*} \left[k^*(x, y, z) h^*(x, y, z) \frac{\partial H^*(x, y, z, t)}{\partial x^*} \right] + \\ & + \frac{\partial}{\partial y^*} \left[k^*(x, y, z) h^*(x, y, z) \frac{\partial H^*(x, y, z, t)}{\partial y^*} \right] + \\ & + \frac{\partial}{\partial z^*} \left[k^*(x, y, z) h^*(x, y, z) \frac{\partial H^*(x, y, z, t)}{\partial z^*} \right] + \\ & + F_1^*(x, y, z, t) - F_2^*(x, y, z, t), \quad [x, y, z] \in G, \end{aligned} \quad (9)$$

with initial condation:

$$H^*(x, y, z, t) = H^{*0}(x, y, z), \quad t = 0, \quad (10)$$

and boundary conditions:

$$k^*(x, y, z) \frac{\partial H^*(x, y, z, t)}{\partial x^*} \Big|_{x=0} = -\alpha_1 \xi^* (H^* - H_0^*), \quad (11)$$

$$k(x, y, z) \frac{\partial H^*(x, y, z, t)}{\partial x^*} \Big|_{x=L_x} = \alpha_1 \xi^* (H^* - H_0^*), \quad (12)$$

$$k^*(x, y, z) \frac{\partial H^*(x, y, z, t)}{\partial y^*} \Big|_{y=0} = -\alpha_2 \xi^* (H^* - H_0^*), \quad (13)$$

$$k^*(x, y, z) \frac{\partial H^*(x, y, z, t)}{\partial y^*} \Big|_{y=L_y} = \alpha_2 \xi^* (H^* - H_0^*), \quad (14)$$

$$\frac{\partial H^*(x, y, z, t)}{\partial z^*} \Big|_{z=0} = 0, \quad (15)$$

$$k^*(x, y, z) \frac{\partial H^*(x, y, z, t)}{\partial z^*} \Big|_{z=L_z} = \alpha_3 \xi^* (H^* - H_0^*). \quad (16)$$

Later, to simplify the problem, we drop the "*" sign in the variable and express the equations (9) – (16) as follows:

$$\begin{aligned} & \beta m(x, y, z) h(x, y, z) \frac{\partial H(x, y, z, t)}{\partial t} = \frac{\partial}{\partial x} \left[k(x, y, z) h(x, y, z) \frac{\partial H(x, y, z, t)}{\partial x} \right] + \\ & + \frac{\partial}{\partial y} \left[k(x, y, z) h(x, y, z) \frac{\partial H(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[k(x, y, z) h(x, y, z) \frac{\partial H(x, y, z, t)}{\partial z} \right] + \\ & + F_1(x, y, z, t) - F_2(x, y, z, t), \quad [x, y, z] \in G, \end{aligned} \quad (17)$$

with initial condation:

$$H(x, y, z, t) = H^0(x, y, z), \quad t = 0, \quad (18)$$

and boundary conditions:

$$k(x, y, z) \frac{\partial H(x, y, z, t)}{\partial x} \Big|_{x=0} = -\alpha_1 \xi (H - H_0), \quad (19)$$

$$k(x, y, z) \frac{\partial H(x, y, z, t)}{\partial x} \Big|_{x=L_x} = \alpha_1 \xi(H - H_0), \quad (20)$$

$$k(x, y, z) \frac{\partial H(x, y, z, t)}{\partial y} \Big|_{y=0} = -\alpha_2 \xi(H - H_0), \quad (21)$$

$$k(x, y, z) \frac{\partial H(x, y, z, t)}{\partial y} \Big|_{y=L_y} = \alpha_2 \xi(H - H_0), \quad (22)$$

$$\frac{\partial H(x, y, z, t)}{\partial z} \Big|_{z=0} = 0, \quad (23)$$

$$k(x, y, z) \frac{\partial H(x, y, z, t)}{\partial z} \Big|_{z=L_z} = \alpha_3 \xi(H - H_0). \quad (24)$$

The convective-diffusion equation of the spread of injected acid in the area with injection wells:

$$\begin{aligned} m_g \frac{\partial C_1(x, y, z, t)}{\partial t} = & \frac{\partial}{\partial x} \left[D_{xx}(x, y, z) \frac{\partial C_1(x, y, z, t)}{\partial x} + \right. \\ & + D_{xy}(x, y, z) \frac{\partial C_1(x, y, z, t)}{\partial y} + D_{xz}(x, y, z) \frac{\partial C_1(x, y, z, t)}{\partial z} \Big] + \\ & + \frac{\partial}{\partial y} \left[D_{yy}(x, y, z) \frac{\partial C_1(x, y, z, t)}{\partial y} + D_{yx}(x, y, z) \frac{\partial C_1(x, y, z, t)}{\partial x} + \right. \\ & + D_{yz}(x, y, z) \frac{\partial C_1(x, y, z, t)}{\partial z} \Big] + \frac{\partial}{\partial z} \left[D_{zz}(x, y, z) \frac{\partial C_1(x, y, z, t)}{\partial z} + \right. \\ & + D_{zx}(x, y, z) \frac{\partial C_1(x, y, z, t)}{\partial x} + D_{zy}(x, y, z) \frac{\partial C_1(x, y, z, t)}{\partial y} \Big] - \\ & - \frac{\partial(V_x(x, y, z, t)C_1(x, y, z, t))}{\partial x} - \frac{\partial(V_y(x, y, z, t)C_1(x, y, z, t))}{\partial y} - \\ & - \frac{\partial(V_z(x, y, z, t)C_1(x, y, z, t))}{\partial z}, \quad [x, y, z] \in G. \end{aligned} \quad (25)$$

with initial condation:

$$C_1(x, y, z, t) = 0, \quad t = 0, \quad (26)$$

boundary condation:

$$C_1(x, y, z, t) = 0, \quad (x, y, z) \in G_k, \quad (27)$$

and wells inside conditions with :

$$C_1(x, y, z, t) = C_{3i}, \quad (x, y, z) \in G_0, \quad (28)$$

$$\left(\frac{\partial C_1(x, y, z, t)}{\partial x} \right)^2 + \left(\frac{\partial C_1(x, y, z, t)}{\partial y} \right)^2 + \left(\frac{\partial C_1(x, y, z, t)}{\partial z} \right)^2 = 0, \quad (x, y, z) \in G_u. \quad (29)$$

The desired concentration distribution of the mixture is determined by solving the following equation:

$$\begin{aligned}
& m_c \frac{\partial C_2(x, y, z, t)}{\partial t} + \frac{\partial N}{\partial t} = \\
& = \frac{\partial}{\partial x} \left[D_{xx}(x, y, z) \frac{\partial C_2(x, y, z, t)}{\partial x} + D_{xy}(x, y, z) \frac{\partial C_2(x, y, z, t)}{\partial y} + \right. \\
& + D_{xz}(x, y, z) \frac{\partial C_2(x, y, z, t)}{\partial z} \left. \right] + \frac{\partial}{\partial y} \left[D_{yy}(x, y, z) \frac{\partial C_2(x, y, z, t)}{\partial y} + \right. \\
& + D_{yx}(x, y, z) \frac{\partial C_2(x, y, z, t)}{\partial x} + D_{yz}(x, y, z) \frac{\partial C_2(x, y, z, t)}{\partial z} \left. \right] + \\
& + \frac{\partial}{\partial z} \left[D_{zz}(x, y, z) \frac{\partial C_2(x, y, z, t)}{\partial z} + D_{zx}(x, y, z) \frac{\partial C_2(x, y, z, t)}{\partial x} + \right. \\
& + D_{zy}(x, y, z) \frac{\partial C_2(x, y, z, t)}{\partial y} \left. \right] - \frac{\partial(V_x(x, y, z, t)C_2(x, y, z, t))}{\partial x} - \\
& - \frac{\partial(V_y(x, y, z, t)C_2(x, y, z, t))}{\partial y} - \frac{\partial(V_z(x, y, z, t)C_2(x, y, z, t))}{\partial z}, \\
& [x, y, z] \in G,
\end{aligned} \tag{30}$$

with initial condation:

$$C_2(x, y, z, t) = C_2^0, \quad t = 0, \tag{31}$$

boundary conditions:

$$\left. \frac{\partial C_2(x, y, z, t)}{\partial x} \right|_{x=0} = -\frac{\alpha_1}{l} (C_2 - C_2^0), \tag{32}$$

$$\left. \frac{\partial C_2(x, y, z, t)}{\partial x} \right|_{x=L_x} = \frac{\alpha_1}{l} (C_2 - C_2^0), \tag{33}$$

$$\left. \frac{\partial C_2(x, y, z, t)}{\partial y} \right|_{y=0} = -\frac{\alpha_2}{l} (C_2 - C_2^0), \tag{34}$$

$$\left. \frac{\partial C_2(x, y, z, t)}{\partial y} \right|_{y=L_y} = \frac{\alpha_2}{l} (C_2 - C_2^0), \tag{35}$$

$$\left. \frac{\partial C_2(x, y, z, t)}{\partial z} \right|_{z=0} = 0, \tag{36}$$

$$\left. \frac{\partial C_2(x, y, z, t)}{\partial z} \right|_{z=L_z} = \frac{\alpha_3}{l} (C_2 - C_2^0), \tag{37}$$

and as well as wells inside conditions:

$$C_2(x, y, z, t) = C_{4i}, \quad (x, y, z) \in G_0, \tag{38}$$

$$\left(\frac{\partial C_2(x, y, z, t)}{\partial x} \right)^2 + \left(\frac{\partial C_2(x, y, z, t)}{\partial y} \right)^2 + \left(\frac{\partial C_2(x, y, z, t)}{\partial z} \right)^2 = 0, \quad (x, y, z) \in G_u. \tag{39}$$

As dimensionless variables are introduced to solve problems (1)–(8) numerically, we reduce equations (25)–(39) to dimensionless variables using the finite difference method, and for simplicity, we omit this process.

The substance one out of phase to the second passage speed defining mass exchange kinetics equation following to appear has:

$$\frac{\partial N(x, y, t)}{\partial t} = \gamma(C_1)f(C_2, N, t), \tag{40}$$

$$N(x, y, t) = N^0(x, y), \quad t = 0, \quad [x, y] \in G. \quad (41)$$

where: C_1 – the concentration of the fuel liquid, C_2 – the concentration of the resulting mixture, $D_{xx}, D_{xy}, D_{xz}, D_{yx}, D_{yy}, D_{yz}, D_{zx}, D_{zy}, D_{zz}$ – filtration coefficients corresponding to x, y, z , (m^2/day), N – process kinetics, γ – mass density of the solution, (kg/m^2); – coefficient of equalization of dimensions of equations, (m); V_x, V_y, V_z – filtration rates respectively by Ox, Oy and Oz axes (m/day), and filtration rates are determined by Darcy's law:

$$V_x(x, y, z, t) = -k(x, y, z) \frac{\partial H(x, y, z, t)}{\partial x}, \quad (42)$$

$$V_y(x, y, z, t) = -k(x, y, z) \frac{\partial H(x, y, z, t)}{\partial y}, \quad (43)$$

$$V_z(x, y, z, t) = -k(x, y, z) \frac{\partial H(x, y, z, t)}{\partial z}. \quad (44)$$

3 Algorithm of problem solving

Because of complexity of given problem, it is difficult to find analytical solution. herefore, we exchange continuous area of problem to grid area as following:

$$\Omega_{xyz} = \{(x_i = i\Delta x, y_j = j\Delta y, z_k = k\Delta z); i = \overline{1, N}; j = \overline{1, M}, k = \overline{1, L}\}$$

and to transfer equation (1) to a finite-difference problem, an algorithmic concept of a variable-direction uncertainty scheme (longitudinal-conduit scheme) is used. The transition from the n – th time layer to the $n + 1$ – th layer is performed in three stages with a step of $1/3$. This as a result three finite difference equations system step-by-step solution is taken. These solutions for $n + 1/3$ – in the layer first limited different equation following the form will take.

Approximation of the equation in the $n+1/3$ layer with respect to the axis Ox :

$$\begin{aligned} & \frac{\beta m_{i,j,k} h_{i,j,k} (H_{i,j,k}^{n+1/3} - H_{i,j,k}^n)}{\Delta \tau / 3} = \\ & = \frac{\varkappa_{i-0.5,j,k} h_{i-0.5,j,k} H_{i-1,j,k}^{n+1/3} - (\varkappa_{i-0.5,j,k} h_{i-0.5,j,k} + \varkappa_{i+0.5,j,k} h_{i+0.5,j,k}) H_{i,j,k}^{n+1/3} + \varkappa_{i+0.5,j,k} h_{i+0.5,j,k} H_{i+1,j,k}^{n+1/3}}{\Delta x^2} + \\ & + \frac{\varkappa_{i,j-0.5,k} h_{i,j-0.5,k} H_{i,j-1,k}^n - (\varkappa_{i,j-0.5,k} h_{i,j-0.5,k} + \varkappa_{i,j+0.5,k} h_{i,j+0.5,k}) H_{i,j,k}^n + \varkappa_{i,j+0.5,k} h_{i,j+0.5,k} H_{i,j+1,k}^n}{\Delta y^2} + \\ & + \frac{\varkappa_{i,j,k-0.5} h_{i,j,k-0.5} H_{i,j,k-1}^n - (\varkappa_{i,j,k-0.5} h_{i,j,k-0.5} + \varkappa_{i,j,k+0.5} h_{i,j,k+0.5}) H_{i,j,k}^n + \varkappa_{i,j,k+0.5} h_{i,j,k+0.5} H_{i,j,k+1}^n}{\Delta z^2} + \\ & + \frac{F_{1,i,j,k}}{3} - \frac{F_{2,i,j,k}}{3} \end{aligned}$$

via grouping similar elements, we get a system of tridiagonal algebraic equations:

$$a_{i,j,k} H_{i-1,j,k}^{n+1/3} - b_{i,j,k} H_{i,j,k}^{n+1/3} + c_{i,j,k} H_{i+1,j,k}^{n+1/3} = -f_{i,j,k}, \quad (45)$$

$$\text{here: } a_{i,j,k} = \frac{\varkappa_{i-0.5,j,k} h_{i-0.5,j,k}}{\Delta x^2}, \quad b_{i,j,k} = \frac{\beta m_{i,j,k} h_{i,j,k}}{\Delta \tau / 3} + \frac{\varkappa_{i-0.5,j,k} h_{i-0.5,j,k} + \varkappa_{i+0.5,j,k} h_{i+0.5,j,k}}{\Delta x^2},$$

$$c_{i,j,k} = \frac{\varkappa_{i+0.5,j,k} h_{i+0.5,j,k}}{\Delta x^2},$$

$$\begin{aligned} f_{i,j,k} = & \frac{\varkappa_{i,j-0.5,k} h_{i,j-0.5,k} H_{i,j-1,k}^n - (\varkappa_{i,j-0.5,k} h_{i,j-0.5,k} + \varkappa_{i,j+0.5,k} h_{i,j+0.5,k}) H_{i,j,k}^n + \varkappa_{i,j+0.5,k} h_{i,j+0.5,k} H_{i,j+1,k}^n}{\Delta y^2} + \\ & + \frac{\varkappa_{i,j,k-0.5} h_{i,j,k-0.5} H_{i,j,k-1}^n - (\varkappa_{i,j,k-0.5} h_{i,j,k-0.5} + \varkappa_{i,j,k+0.5} h_{i,j,k+0.5}) H_{i,j,k}^n + \varkappa_{i,j,k+0.5} h_{i,j,k+0.5} H_{i,j,k+1}^n}{\Delta z^2} + \\ & + \frac{\beta m_{i,j,k} h_{i,j,k} H_{i,j,k}^n}{\Delta \tau / 3} + \frac{F_{1,i,j,k}}{3} - \frac{F_{2,i,j,k}}{3}. \end{aligned}$$

(19) boundary condition Ox axis according to approximation as follows we get:

$$\varkappa_{1,j,k} \frac{-3H_{0,j,k}^{n+1/3} + 4H_{1,j,k}^{n+1/3} - H_{2,j,k}^{n+1/3}}{2\Delta x} = -\alpha_1 \xi (H_{1,j,k}^{n+1/3} - H_0). \quad (46)$$

From three diagonal equations system (38) we find $H_{2,j,k}^{n+1/3}$ at $i = 1$:

$$\begin{aligned} a_{1,j,k} H_{0,j,k}^{n+1/3} - b_{1,j,k} H_{1,j,k}^{n+1/3} + c_{1,j,k} H_{2,j,k}^{n+1/3} &= -f_{1,j,k}, \\ H_{2,j,k}^{n+1/3} &= -\frac{a_{1,j,k}}{c_{1,j,k}} H_{0,j,k}^{n+1/3} + \frac{b_{1,j,k}}{c_{1,j,k}} H_{1,j,k}^{n+1/3} - \frac{f_{1,j,k}}{c_{1,j,k}}. \end{aligned} \quad (47)$$

We find $H_{0,j,k}^{n+1/3}$ by substituting $H_{2,j,k}^{n+1/3}$ in (47) into (46):

$$H_{0,j,k}^{n+1/3} = \frac{\varkappa_{1,j,k} b_{1,j,k} - 4\varkappa_{1,j,k} c_{1,j,k} - 2\iota_1 \Delta x \xi c_{1,j,k}}{\varkappa_{1,j,k} a_{1,j,k} - 3\varkappa_{1,j,k} c_{1,j,k}} H_{1,j,k}^{n+1/3} + \frac{2\iota_1 \Delta x \xi c_{1,j,k} H_0 - \varkappa_{1,j,k} f_{1,j,k}}{\varkappa_{1,j,k} a_{1,j,k} - 3\varkappa_{1,j,k} c_{1,j,k}},$$

here $\alpha_{0,j,k}, \beta_{0,j,k}$ coefficients are found by following formula:

$$\alpha_{0,j,k} = \frac{\varkappa_{1,j,k} b_{1,j,k} - 4\varkappa_{1,j,k} c_{1,j,k} - 2\iota_1 \Delta x \xi c_{1,j,k}}{\varkappa_{1,j,k} a_{1,j,k} - 3\varkappa_{1,j,k} c_{1,j,k}}, \quad \beta_{0,j,k} = \frac{2\Delta x \iota_1 \xi c_{1,j,k} H_0 - \varkappa_{1,j,k} f_{1,j,k}}{\varkappa_{1,j,k} a_{1,j,k} - 3\varkappa_{1,j,k} c_{1,j,k}}.$$

As above, we obtain follows from the approximation of (20) the boundary condition with respect to Ox :

$$\varkappa_{N,j,k} \frac{H_{N-2,j,k}^{n+1/3} - 4H_{N-1,j,k}^{n+1/3} + 3H_{N,j,k}^{n+1/3}}{2\Delta x} = -\alpha_1 \xi (H_{N-1,j,k}^{n+1/3} - H_0). \quad (48)$$

Using sweep method, at $N, N-1$ and $N-2$, we find $H_{N-1,j,k}^{n+1/3}$ and $H_{N-2,j,k}^{n+1/3}$:

$$H_{N-1,j,k}^{n+1/3} = \alpha_{N-1,j,k} H_{N,j,k}^{n+1/3} + \beta_{N-1,j,k}, \quad (49)$$

$$\begin{aligned} H_{N-2,j,k}^{n+1/3} &= \alpha_{N-2,j,k} H_{N-1,j,k}^{n+1/3} + \beta_{N-2,j,k} = \\ &= \alpha_{N-2,j,k} \alpha_{N-1,j,k} H_{N,j,k}^{n+1/3} + \alpha_{N-2,j,k} \beta_{N-1,j,k} + \beta_{N-2,j,k}. \end{aligned} \quad (50)$$

We find $H_{N,j,k}^{n+1/3}$ by substituting $H_{N-1,j,k}^{n+1/3}$ in (49) and $H_{N-2,j,k}^{n+1/3}$ in (50) into (47):

$$\begin{aligned} H_{N,j,k}^{n+1/3} &= \\ &= \frac{4\beta_{N-1,j,k} \varkappa_{N,j,k} - 2\iota_1 \xi \Delta x \beta_{N-1,j,k} + 2\iota_1 \xi \Delta x H_0 - \alpha_{N-2,j,k} \beta_{N-1,j,k} \varkappa_{N,j,k} - \beta_{N-2,j,k} \varkappa_{N,j,k}}{\alpha_{N-2,j,k} \alpha_{N-1,j,k} \varkappa_{N,j,k} + 3\varkappa_{N,j,k} - 4\alpha_{N-1,j,k} \varkappa_{N,j,k} + 2\iota_1 \xi \Delta x \alpha_{N-1,j,k}}. \end{aligned} \quad (51)$$

$H_{N-1,j,k}^{n+1/3}, H_{N-2,j,k}^{n+1/3}, \dots, H_{1,j,k}^{n+1/3}$ pressure values are connected to each others by following:

$$H_{i,j,k}^{n+1/3} = \alpha_{i,j,k} H_{i+1,j,k}^{n+1/3} + \beta_{i,j,k}, \quad i = \overline{N-1, 1}, \quad j = \overline{0, M}, \quad k = \overline{0, L}.$$

As above, we use the finite-difference method to solve equation (1) on the $n+2/3$ time scale, grouping similar terms to obtain a system of tridiagonal algebraic equations with respect to the required variables:

$$\bar{a}_{i,j,k} H_{i,j-1,k}^{n+2/3} - \bar{b}_{i,j,k} H_{i,j,k}^{n+2/3} + \bar{c}_{i,j,k} H_{i,j+1,k}^{n+2/3} = -\bar{f}_{i,j,k}, \quad (52)$$

here: $\bar{a}_{i,j,k} = \frac{\varkappa_{i,j-0.5,k} h_{i,j-0.5,k}}{\Delta y^2}$, $\bar{b}_{i,j,k} = \frac{\beta m_{i,j,k} h_{i,j,k}}{\Delta \tau/3} + \frac{\varkappa_{i,j-0.5,k} h_{i,j-0.5,k} + \varkappa_{i,j+0.5,k} h_{i,j+0.5,k}}{\Delta y^2}$,

$$\bar{c}_{i,j,k} = \frac{\varkappa_{i,j+0.5,k} h_{i,j+0.5,k}}{\Delta y^2},$$

$$\bar{f}_{i,j,k} = \frac{\varkappa_{i-0.5,j,k} h_{i-0.5,j,k} H_{i-1,j,k}^{n+1/3} - (\varkappa_{i-0.5,j,k} h_{i-0.5,j,k} + \varkappa_{i+0.5,j,k} h_{i+0.5,j,k}) H_{i,j,k}^{n+1/3} + \varkappa_{i+0.5,j,k} h_{i+0.5,j,k} H_{i+1,j,k}^{n+1/3}}{\Delta x^2} +$$

$$\frac{\varkappa_{i,j,k-0.5} h_{i,j,k-0.5} H_{i,j,k-1}^{n+1/3} - (\varkappa_{i,j,k-0.5} h_{i,j,k-0.5} + \varkappa_{i,j,k+0.5} h_{i,j,k+0.5}) H_{i,j,k}^{n+1/3} + \varkappa_{i,j,k+0.5} h_{i,j,k+0.5} H_{i,j,k+1}^{n+1/3}}{\Delta z^2} +$$

$$+ \frac{\beta m_{i,j,k} h_{i,j,k} H_{i,j,k}^{n+1/3}}{\Delta \tau/3} + \frac{F_{1,i,j,k}}{3} - \frac{F_{2,i,j,k}}{3}.$$

As above, we obtain follows from the approximation of (21) the boundary condition with respect to Oy :

$$\varkappa_{i,1,k} \frac{-3H_{i,0,k}^{n+2/3} + 4H_{i,1,k}^{n+2/3} - H_{i,2,k}^{n+2/3}}{2\Delta y} = -\alpha_2 \xi (H_{i,1,k}^{n+2/3} - H_0), \quad (53)$$

we find $H_{i,2,k}^{n+2/3}$ via the system of tridiagonal equations (52) at $j = 1$:

$$\bar{a}_{i,1,k} H_{i,0,k}^{n+2/3} - \bar{b}_{i,1,k} H_{i,1,k}^{n+2/3} + \bar{c}_{i,1,k} H_{i,2,k}^{n+2/3} = -\bar{f}_{i,1,k}, \quad (54)$$

$$H_{i,2,k}^{n+2/3} = -\frac{\bar{a}_{i,1,k}}{\bar{c}_{i,1,k}} H_{i,0,k}^{n+2/3} + \frac{\bar{b}_{i,1,k}}{\bar{c}_{i,1,k}} H_{i,1,k}^{n+2/3} - \frac{\bar{f}_{i,1,k}}{\bar{c}_{i,1,k}}, \quad (55)$$

we get $H_{i,0,k}^{n+2/3}$ by substituting $H_{i,2,k}^{n+2/3}$ in (55) into (53):

$$H_{i,0,k}^{n+2/3} = \frac{\varkappa_{i,1,k} \bar{b}_{i,1,k} - 4\varkappa_{i,1,k} \bar{c}_{i,1,k} - 2\iota_2 \xi \Delta y \bar{c}_{i,1,k} H_{i,1,k}^{n+2/3} + \frac{2\iota_2 \xi \Delta y \bar{c}_{i,1,k} H_0 - \varkappa_{i,1,k} \bar{f}_{i,1,k}}{\varkappa_{i,1,k} \bar{a}_{i,1,k} - 3\varkappa_{i,1,k} \bar{c}_{i,1,k}}}.$$

Sweep method coefficients $\bar{\alpha}_{i,0,k}$ and $\bar{\beta}_{i,0,k}$ are calculated by the following formula:

$$\bar{\alpha}_{i,0,k} = \frac{\varkappa_{i,1,k} \bar{b}_{i,1,k} - 4\varkappa_{i,1,k} \bar{c}_{i,1,k} - 2\iota_2 \xi \Delta y \bar{c}_{i,1,k}}{\varkappa_{i,1,k} \bar{a}_{i,1,k} - 3\varkappa_{i,1,k} \bar{c}_{i,1,k}}, \quad \bar{\beta}_{i,0,k} = \frac{2\iota_2 \xi \Delta y \bar{c}_{i,1,k} H_0 - \varkappa_{i,1,k} \bar{f}_{i,1,k}}{\varkappa_{i,1,k} \bar{a}_{i,1,k} - 3\varkappa_{i,1,k} \bar{c}_{i,1,k}}.$$

As above we obtain follows from the approximation of (22) the boundary condition with respect to Oy :

$$\varkappa_{i,N,k} \frac{H_{i,N-2,k}^{n+2/3} - 4H_{i,N-1,k}^{n+2/3} + 3H_{i,N,k}^{n+2/3}}{2\Delta y} = -\alpha_2 \xi (H_{i,N-1,k}^{n+2/3} - H_0). \quad (56)$$

Using sweep method, at $N, N-1$ and $N-2$, we find $H_{i,N-1,k}^{n+2/3}$ and $H_{i,N-2,k}^{n+2/3}$:

$$H_{i,N-1,k}^{n+2/3} = \bar{\alpha}_{i,N-1,k} H_{i,N,k}^{n+2/3} + \bar{\beta}_{i,N-1,k}, \quad (57)$$

$$H_{i,N-2,k}^{n+2/3} = \bar{\alpha}_{i,N-2,k} H_{i,N-1,k}^{n+2/3} + \bar{\beta}_{i,N-2,k} =$$

$$= \bar{\alpha}_{i,N-2,k} \bar{\alpha}_{i,N-1,k} H_{i,N,k}^{n+2/3} + \bar{\alpha}_{i,N-2,k} \bar{\beta}_{i,N-1,k} + \bar{\beta}_{i,N-2,k}. \quad (58)$$

We find $H_{i,N,k}^{n+2/3}$ by substituting $H_{i,N-1,k}^{n+2/3}$ in (57) and $H_{i,N-2,k}^{n+2/3}$ in (58) into (56):

$$H_{i,N,k}^{n+2/3} =$$

$$= \frac{4\bar{\beta}_{i,N-1,k} \varkappa_{i,N,k} - 2\iota_2 \xi \Delta y \bar{\beta}_{i,N-1,k} + 2\iota_2 \xi \Delta y H_0 - \bar{\alpha}_{i,N-2,k} \bar{\beta}_{i,N-1,k} \varkappa_{i,N,k} - \bar{\beta}_{i,N-2,k} \varkappa_{i,N,k}}{\bar{\alpha}_{i,N-2,k} \bar{\alpha}_{i,N-1,k} \varkappa_{i,N,k} + 3\varkappa_{i,N,k} - 4\bar{\alpha}_{i,N-1,k} \varkappa_{i,N,k} + 2\iota_2 \xi \Delta y \bar{\alpha}_{i,N-1,k}}.$$

$H_{i,N-1,k}^{n+2/3}, H_{i,N-1,k}^{n+2/3}, \dots, H_{i,1,k}^{n+2/3}$ pressure values are connected to each others by following:

$$H_{i,j,k}^{n+2/3} = \bar{\alpha}_{i,j,k} H_{i,j+1,k}^{n+2/3} + \bar{\beta}_{i,j,k}, \quad i = \overline{0, M}, \quad j = \overline{N-1, 1}, \quad k = \overline{0, L}.$$

As above, we use the finite-difference method to solve equation (1) on the $n+1$ time scale, grouping similar terms to obtain a system of tridiagonal algebraic equations with respect to the required variables:

$$\bar{a}_{i,j,k} H_{i,j,k-1}^{n+1} - \bar{b}_{i,j,k} H_{i,j,k}^{n+1} + \bar{c}_{i,j,k} H_{i,j,k+1}^{n+1} = -\bar{f}_{i,j,k}, \quad (59)$$

$$\text{here : } \bar{a}_{i,j,k} = \frac{\varkappa_{i,j,k-0.5} h_{i,j,k-0.5} H_{i,j,k-1}^{n+1}}{\Delta z^2}, \quad \bar{b}_{i,j,k} = \frac{\beta m_{i,j,k} h_{i,j,k}}{\Delta \tau / 3} + \frac{\varkappa_{i,j,k-0.5} h_{i,j,k-0.5} + \varkappa_{i,j,k+0.5} h_{i,j,k+0.5}}{\Delta z^2},$$

$$\bar{c}_{i,j,k} = \frac{\varkappa_{i,j,k+0.5} h_{i,j,k+0.5}}{\Delta z^2},$$

$$\begin{aligned} \bar{f}_{i,j,k} = & \frac{\varkappa_{i-0.5,j,k} h_{i-0.5,j,k} H_{i-1,j,k}^{n+2/3} - (\varkappa_{i-0.5,j,k} h_{i-0.5,j,k} + \varkappa_{i+0.5,j,k} h_{i+0.5,j,k}) H_{i,j,k}^{n+2/3} + \varkappa_{i+0.5,j,k} h_{i+0.5,j,k} H_{i+1,j,k}^{n+2/3}}{\Delta x^2} + \\ & + \frac{\varkappa_{i,j-0.5,k} h_{i,j-0.5,k} H_{i,j-1,k}^{n+2/3} - (\varkappa_{i,j-0.5,k} h_{i,j-0.5,k} + \varkappa_{i,j+0.5,k} h_{i,j+0.5,k}) H_{i,j,k}^{n+2/3} + \varkappa_{i,j+0.5,k} h_{i,j+0.5,k} H_{i,j+1,k}^{n+2/3}}{\Delta y^2} + \\ & + \frac{\beta m_{i,j,k} h_{i,j,k} H_{i,j,k}^{n+2/3}}{\Delta \tau / 3} + \frac{F_{1,i,j,k}}{3} - \frac{F_{2,i,j,k}}{3}. \end{aligned}$$

As above, we obtain follows from the approximation of (23) the boundary condition with respect to Oz :

$$-3H_{i,j,0}^{n+1} + 4H_{i,j,1}^{n+1} - H_{i,j,2}^{n+1} = 0, \quad (60)$$

we find $H_{i,j,2}^{n+1}$ via the system of tridiagonal equations (59) at $k=1$:

$$\begin{aligned} \bar{a}_{i,j,1} H_{i,j,0}^{n+1} - \bar{b}_{i,j,1} H_{i,j,1}^{n+1} + \bar{c}_{i,j,1} H_{i,j,2}^{n+1} &= -\bar{f}_{i,j,1}, \\ H_{i,j,2}^{n+1} &= -\frac{\bar{a}_{i,j,1}}{\bar{c}_{i,j,1}} H_{i,j,0}^{n+1} + \frac{\bar{b}_{i,j,1}}{\bar{c}_{i,j,1}} H_{i,j,1}^{n+1} - \frac{\bar{f}_{i,j,1}}{\bar{c}_{i,j,1}}, \end{aligned} \quad (61)$$

we take $H_{i,j,0}^{n+1}$ by substituting $H_{i,j,2}^{n+1}$ in (60) into (60):

$$H_{i,j,0}^{n+1} = \frac{(4\bar{c}_{i,j,1} - \bar{b}_{i,j,1})}{(3\bar{c}_{i,j,1} - \bar{a}_{i,j,1})} H_{i,j,1}^{n+1} + \frac{\bar{f}_{i,j,1}}{(3\bar{c}_{i,j,1} - \bar{a}_{i,j,1})}.$$

Sweep method coefficients $\bar{\alpha}_{i,0,k}$ and $\bar{\beta}_{i,0,k}$ are calculated by the following formula:

$$\bar{\alpha}_{i,j,0} = \frac{(4\bar{c}_{i,j,1} - \bar{b}_{i,j,1})}{(3\bar{c}_{i,j,1} - \bar{a}_{i,j,1})}, \quad \bar{\beta}_{i,j,0} = \frac{\bar{f}_{i,j,1}}{(3\bar{c}_{i,j,1} - \bar{a}_{i,j,1})}.$$

As above, we obtain follows from the approximation of (24) the boundary condition with respect to Oz :

$$\varkappa_{i,j,N} \frac{H_{i,j,N-2}^{n+1} - 4H_{i,j,N-1}^{n+1} + 3H_{i,j,N}^{n+1}}{2\Delta z} = -\iota_3 \xi (H_{i,j,N-1}^{n+1} - H_0). \quad (62)$$

Using sweep method, at $N, N-1$ and $N-2$, we find $H_{i,j,N-1}^{n+1}$ and $H_{i,j,N-2}^{n+1}$:

$$H_{i,j,N-1}^{n+1} = \bar{\alpha}_{i,j,N-1} H_{i,j,N}^{n+1} + \bar{\beta}_{i,j,N-1}, \quad (63)$$

$$\begin{aligned}
H_{i,j,N-2}^{n+1} &= \bar{\alpha}_{i,j,N-2} H_{i,j,N-1}^{n+1} + \bar{\beta}_{i,j,N-2} = \\
&= \bar{\alpha}_{i,j,N-2} \bar{\alpha}_{i,j,N-1} H_{i,j,N}^{n+1} + \bar{\alpha}_{i,j,N-2} \bar{\beta}_{i,j,N-1} + \bar{\beta}_{i,j,N-2}.
\end{aligned} \tag{64}$$

We find $H_{i,j,N}^{n+1}$ by substituting $H_{i,j,N-1}^{n+1}$ in (63) and $H_{i,j,N-2}^{n+1}$ in (64) into (62):

$$\begin{aligned}
H_{i,j,N}^{n+1} &= \\
&= \frac{4\bar{\beta}_{i,j,N-1} \chi_{i,j,N} - 2\iota_3 \xi \Delta z \bar{\beta}_{i,j,N-1} + 2\iota_3 \xi \Delta z H_0 - \bar{\alpha}_{i,j,N-2} \bar{\beta}_{i,j,N-1} \chi_{i,N,k} - \bar{\beta}_{i,j,N-2} \chi_{i,j,N}}{\bar{\alpha}_{i,j,N-2} \bar{\alpha}_{i,j,N-1} \chi_{i,j,N} + 3\chi_{i,j,N} - 4\bar{\alpha}_{i,j,N-1} \chi_{i,j,N} + 2\iota_3 \xi \Delta z \bar{\alpha}_{i,j,N-1}}.
\end{aligned}$$

$H_{i,j,N-1}^{n+1}, H_{i,j,N-1}^{n+1}, \dots, H_{i,j,1}^{n+1}$ pressure values are connected to each others by following:

$$H_{i,j,k}^{n+1} = \bar{\alpha}_{i,j,k} H_{i,j,k+1}^{n+1} + \bar{\beta}_{i,j,k}, \quad i = \overline{0, L}, \quad j = \overline{0, M}, \quad k = \overline{N-1, 1}.$$

As in the pressure equation, in the first concentration equation, the partial derivatives for the three layers are solved by the finite difference method, and the system of tridiagonal equations is solved using the coefficients of the drive. these works are presented in the article [3]. For convenience, we present calculations for the first layer.

For the $n + 1/3$ layer, we replace the differential equation with a finite difference equation and obtain equations (28) for numerical integration.

$$\begin{aligned}
m_g \frac{C_{1,i,j,k}^{n+1/3} - C_{1,i,j,k}^n}{\Delta \tau / 3} &= \frac{D_{11,i-0.5,j,k} C_{1,i-1,j,k}^{n+1/3} - (D_{11,i-0.5,j,k} + D_{11,i+0.5,j,k}) C_{1,i,j,k}^{n+1/3} + D_{11,i+0.5,j,k} C_{1,i+1,j,k}^{n+1/3}}{\Delta x^2} + \\
&+ \frac{D_{12,i-0.5,j,k} C_{1,i-1,j-1,k}^n - D_{12,i-0.5,j,k} C_{1,i-1,j+1,k}^n - D_{12,i+0.5,j,k} C_{1,i+1,j-1,k}^n + D_{12,i+0.5,j,k} C_{1,i+1,j+1,k}^n}{\Delta x \Delta y} + \\
&+ \frac{D_{13,i-0.5,j,k} C_{1,i-1,j,k-1}^n - D_{13,i-0.5,j,k} C_{1,i-1,j,k+1}^n - D_{13,i+0.5,j,k} C_{1,i+1,j,k-1}^n + D_{13,i+0.5,j,k} C_{1,i+1,j,k+1}^n}{\Delta x \Delta z} + \\
&+ \frac{D_{22,i,j-0.5,k} C_{1,i,j-1,k}^n - (D_{22,i,j-0.5,k} + D_{22,i,j+0.5,k}) C_{1,i,j,k}^n + D_{22,i,j+0.5,k} C_{1,i,j+1,k}^n}{\Delta y^2} + \\
&+ \frac{D_{21,i,j-0.5,k} C_{1,i-1,j-1,k}^n - D_{21,i,j-0.5,k} C_{1,i-1,j+1,k}^n - D_{21,i,j+0.5,k} C_{1,i+1,j-1,k}^n + D_{21,i,j+0.5,k} C_{1,i+1,j+1,k}^n}{\Delta x \Delta y} + \\
&+ \frac{D_{23,i,j-0.5,k} C_{1,i,j-1,k-1}^n - D_{23,i,j-0.5,k} C_{1,i,j-1,k+1}^n - D_{23,i,j+0.5,k} C_{1,i,j+1,k-1}^n + D_{23,i,j+0.5,k} C_{1,i,j+1,k+1}^n}{\Delta y \Delta z} + \\
&+ \frac{D_{33,i,j,k-0.5} C_{1,i,j,k-1}^n - (D_{33,i,j,k-0.5} + D_{33,i,j,k+0.5}) C_{1,i,j,k}^n + D_{33,i,j,k+0.5} C_{1,i,j,k+1}^n}{\Delta z^2} + \\
&+ \frac{D_{31,i,j-0.5,k} C_{1,i-1,j,k-1}^n - D_{31,i,j-0.5,k} C_{1,i-1,j,k+1}^n - D_{31,i,j+0.5,k} C_{1,i+1,j,k-1}^n + D_{31,i,j+0.5,k} C_{1,i+1,j,k+1}^n}{\Delta x \Delta z} + \\
&+ \frac{D_{32,i,j,k-0.5} C_{1,i,j-1,k-1}^n - D_{32,i,j,k-0.5} C_{1,i,j-1,k+1}^n - D_{32,i,j,k+0.5} C_{1,i,j+1,k-1}^n + D_{32,i,j,k+0.5} C_{1,i,j+1,k+1}^n}{\Delta y \Delta z} + \\
&+ \frac{V_{1,i-0.5,j,k} C_{1,i-1,j,k}^n - V_{1,i+0.5,j,k} C_{1,i+1,j,k}^n}{2\Delta x} + \frac{V_{2,i,j-0.5,k} C_{1,i,j-1,k}^n - V_{2,i,j+0.5,k} C_{1,i,j+1,k}^n}{2\Delta y} + \\
&+ \frac{V_{3,i,j,k-0.5} C_{1,i,j,k-1}^n - V_{3,i,j,k+0.5} C_{1,i,j,k+1}^n}{2\Delta z},
\end{aligned}$$

and after grouping this equation, we get:

$$a'_{i,j,k} C_{1,i-1,j,k}^{n+1/3} - b'_{i,j,k} C_{1,i,j,k}^{n+1/3} + c'_{i,j,k} C_{1,i+1,j,k}^{n+1/3} = -f'_{i,j,k}, \tag{65}$$

here : $a'_{i,j,k} = \frac{D_{11,i-0.5,j,k}}{\Delta x^2}$, $b'_{i,j,k} = \frac{m_g}{\Delta \tau / 3} + \frac{(D_{11,i-0.5,j,k} + D_{11,i+0.5,j,k})}{\Delta x^2}$, $c'_{i,j,k} = \frac{D_{11,i+0.5,j,k}}{\Delta x^2}$,

$$\begin{aligned}
f'_{i,j,k} &= \frac{D_{12,i-0.5,j,k} C_{1,i-1,j-1,k}^n - D_{12,i-0.5,j,k} C_{1,i-1,j+1,k}^n - D_{12,i+0.5,j,k} C_{1,i+1,j-1,k}^n + D_{12,i+0.5,j,k} C_{1,i+1,j+1,k}^n}{\Delta x \Delta y} + \\
&+ \frac{D_{13,i-0.5,j,k} C_{1,i-1,j,k-1}^n - D_{13,i-0.5,j,k} C_{1,i-1,j,k+1}^n - D_{13,i+0.5,j,k} C_{1,i+1,j,k-1}^n + D_{13,i+0.5,j,k} C_{1,i+1,j,k+1}^n}{\Delta x \Delta z} + \\
&+ \frac{D_{22,i,j-0.5,k} C_{1,i,j-1,k}^n - (D_{22,i,j-0.5,k} + D_{22,i,j+0.5,k}) C_{1,i,j,k}^n + D_{22,i,j+0.5,k} C_{1,i,j+1,k}^n}{\Delta y^2} + \\
&+ \frac{D_{21,i,j-0.5,k} C_{1,i-1,j-1,k}^n - D_{21,i,j-0.5,k} C_{1,i-1,j+1,k}^n - D_{21,i,j+0.5,k} C_{1,i+1,j-1,k}^n + D_{21,i,j+0.5,k} C_{1,i+1,j+1,k}^n}{\Delta x \Delta y} +
\end{aligned}$$

$$\begin{aligned}
& + \frac{D_{23,i,j-0.5,k}C_{1,i,j-1,k-1}^n - D_{23,i,j-0.5,k}C_{1,i,j-1,k+1}^n - D_{23,i,j+0.5,k}C_{1,i,j+1,k-1}^n + D_{23,i,j+0.5,k}C_{1,i,j+1,k+1}^n}{\Delta y \Delta z} + \\
& + \frac{D_{33,i,j,k-0.5}C_{1,i,j,k-1}^n - (D_{33,i,j,k-0.5} + D_{33,i,j,k+0.5})C_{1,i,j,k}^n + D_{33,i,j,k+0.5}C_{1,i,j,k+1}^n}{\Delta z^2} + \\
& + \frac{D_{31,i,j-0.5,k}C_{1,i-1,j,k-1}^n - D_{31,i,j-0.5,k}C_{1,i-1,j,k+1}^n - D_{31,i,j+0.5,k}C_{1,i+1,j,k-1}^n + D_{31,i,j+0.5,k}C_{1,i+1,j,k+1}^n}{\Delta x \Delta z} + \\
& + \frac{D_{32,i,j,k-0.5}C_{1,i,j-1,k-1}^n - D_{32,i,j,k-0.5}C_{1,i,j-1,k+1}^n - D_{32,i,j,k+0.5}C_{1,i,j+1,k-1}^n + D_{32,i,j,k+0.5}C_{1,i,j+1,k+1}^n}{\Delta y \Delta z} + \\
& + \frac{V_{1,i-0.5,j,k}C_{1,i-1,j,k}^n - V_{1,i+0.5,j,k}C_{1,i+1,j,k}^n}{2\Delta x} + \frac{V_{2,i,j-0.5,k}C_{1,i,j-1,k}^n - V_{2,i,j+0.5,k}C_{1,i,j+1,k}^n}{2\Delta y} + \\
& + \frac{V_{3,i,j,k-0.5}C_{1,i,j,k-1}^n - V_{3,i,j,k+0.5}C_{1,i,j,k+1}^n}{2\Delta z} + \frac{m_g C_{1,i,j,k}^n}{\Delta \tau / 3}.
\end{aligned}$$

As above, we obtain follows from the approximation of (30) the boundary condition with respect to Ox :

$$\frac{-3C_{1,0,j,k}^{n+1/3} + 4C_{1,1,j,k}^{n+1/3} - C_{1,2,j,k}^{n+1/3}}{2\Delta x} = 0, \quad (66)$$

we find $C_{1,2,j,k}^{n+1/3}$ via the system of tridiagonal equations (52) at $i = 1$:

$$\begin{aligned}
a'_{1,j,k}C_{1,0,j,k}^{n+1/3} - b'_{1,j,k}C_{1,1,j,k}^{n+1/3} + c'_{1,j,k}C_{1,2,j,k}^{n+1/3} &= -f'_{1,j,k}, \\
C_{1,2,j,k}^{n+1/3} &= -\frac{a'_{1,j,k}}{c'_{1,j,k}}C_{1,0,j,k}^{n+1/3} + \frac{b'_{1,j,k}}{c'_{1,j,k}}C_{1,1,j,k}^{n+1/3} - \frac{f'_{1,j,k}}{c'_{1,j,k}}, \quad (67)
\end{aligned}$$

we get $C_{1,0,j,k}^{n+1/3}$ by substituting $C_{1,2,j,k}^{n+1/3}$ in (60) into (59):

$$C_{1,0,j,k}^{n+1/3} = \frac{(b'_{1,j,k} - 4c'_{1,j,k})}{(a'_{1,j,k} - 3c'_{1,j,k})}C_{1,1,j,k}^{n+1/3} + \frac{f'_{1,j,k}}{(3c'_{1,j,k} - a'_{1,j,k})}.$$

Sweep method coefficients and are calculated by following formula:

$$\alpha'_{0,j,k} = \frac{(b'_{1,j,k} - 4c'_{1,j,k})}{(a'_{1,j,k} - 3c'_{1,j,k})}, \quad \beta'_{0,j,k} = \frac{f'_{1,j,k}}{(3c'_{1,j,k} - a'_{1,j,k})}.$$

As above, we obtain follows from the approximation of (32) the boundary condition with respect to Ox :

$$\frac{C_{1,N-2,j,k}^{n+1/3} - 4C_{1,N-1,j,k}^{n+1/3} + 3C_{1,N,j,k}^{n+1/3}}{2\Delta x} = 0. \quad (68)$$

Using sweep method, at $N, N-1$ and $N-2$, we find $C_{1,N-1,j,k}^{n+1/3}$ and $C_{1,N-2,j,k}^{n+1/3}$

$$C_{1,N-1,j,k}^{n+1/3} = \alpha'_{N-1,j,k}C_{1,N,j,k}^{n+1/3} + \beta'_{N-1,j,k}, \quad (69)$$

$$\begin{aligned}
C_{1,N-2,j,k}^{n+1/3} &= \alpha'_{N-2,j,k}C_{1,N-1,j,k}^{n+1/3} + \beta'_{N-2,j,k} = \\
&= \alpha'_{N-2,j,k}\alpha'_{N-1,j,k}C_{1,N,j,k}^{n+1/3} + \alpha'_{N-2,j,k}\beta'_{N-1,j,k} + \beta'_{N-2,j,k}. \quad (70)
\end{aligned}$$

We find $C_{1,N,j,k}^{n+1/3}$ by substituting $C_{1,N-1,j,k}^{n+1/3}$ in (62) and $C_{1,N-2,j,k}^{n+1/3}$ in (63) into (61):

$$C_{1,N,j,k}^{n+1/3} = \frac{4\beta'_{N-1,j,k} - \alpha'_{N-2,j,k}\beta'_{N-1,j,k} - \beta'_{N-2,j,k}}{\alpha'_{N-2,j,k}\alpha'_{N-1,j,k} - 4\alpha'_{N-1,j,k} + 3}.$$

$$C_{1,N-1,j,k}^{n+1/3}, C_{1,N-2,j,k}^{n+1/3}, \dots, C_{1,1,j,k}^{n+1/3}$$

concentration values are connected to each others by following:

$$C_{1,i,j,k}^{n+1/3} = \alpha'_{i,j,k} C_{1,i+1,j,k}^{n+1/3} + \beta'_{i,j,k}; \quad i = \overline{N-1, 1}, \quad j = \overline{0, M}, \quad k = \overline{0, L}.$$

Above like concentration of the mixture in the equation also three layer according to partial derivatives limited difference in the manner is being answered and propulsive coefficients through three diagonally equations system solved. this works [3] in the article given. For convenience, we present calculations for the first layer.

$n + 1/3$ layer differential equation for finite difference equation with by replacing (33) equations numerical integration for we get:

$$\begin{aligned} m_g \frac{C_{2,i,j,k}^{n+1/3} - C_{2,i,j,k}^n}{\Delta\tau/3} = & \frac{D_{11,i-0.5,j,k} C_{2,i-1,j,k}^{n+1/3} - (D_{11,i-0.5,j,k} + D_{11,i+0.5,j,k}) C_{2,i,j,k}^{n+1/3} + D_{11,i+0.5,j,k} C_{2,i+1,j,k}^{n+1/3}}{\Delta x^2} + \\ & + \frac{D_{12,i-0.5,j,k} C_{2,i-1,j-1,k}^n - D_{12,i-0.5,j,k} C_{2,i-1,j+1,k}^n - D_{12,i+0.5,j,k} C_{2,i+1,j-1,k}^n + D_{12,i+0.5,j,k} C_{2,i+1,j+1,k}^n}{\Delta x \Delta y} + \\ & + \frac{D_{13,i-0.5,j,k} C_{2,i-1,j,k-1}^n - D_{13,i-0.5,j,k} C_{2,i-1,j,k+1}^n - D_{13,i+0.5,j,k} C_{2,i+1,j,k-1}^n + D_{13,i+0.5,j,k} C_{2,i+1,j,k+1}^n}{\Delta x \Delta z} + \\ & + \frac{D_{22,i,j-0.5,k} C_{2,i,j-1,k}^n - (D_{22,i,j-0.5,k} + D_{22,i,j+0.5,k}) C_{2,i,j,k}^n + D_{22,i,j+0.5,k} C_{2,i,j+1,k}^n}{\Delta y^2} + \\ & + \frac{D_{21,i,j-0.5,k} C_{2,i-1,j-1,k}^n - D_{21,i,j-0.5,k} C_{2,i-1,j+1,k}^n - D_{21,i,j+0.5,k} C_{2,i+1,j-1,k}^n + D_{21,i,j+0.5,k} C_{2,i+1,j+1,k}^n}{\Delta x \Delta y} + \\ & + \frac{D_{23,i,j-0.5,k} C_{2,i,j-1,k-1}^n - D_{23,i,j-0.5,k} C_{2,i,j-1,k+1}^n - D_{23,i,j+0.5,k} C_{2,i,j+1,k-1}^n + D_{23,i,j+0.5,k} C_{2,i,j+1,k+1}^n}{\Delta y \Delta z} + \\ & + \frac{D_{33,i,j,k-0.5} C_{2,i,j,k-1}^n - (D_{33,i,j,k-0.5} + D_{33,i,j,k+0.5}) C_{2,i,j,k}^n + D_{33,i,j,k+0.5} C_{2,i,j,k+1}^n}{\Delta z^2} + \\ & + \frac{D_{31,i,j-0.5,k} C_{2,i-1,j,k-1}^n - D_{31,i,j-0.5,k} C_{2,i-1,j,k+1}^n - D_{31,i,j+0.5,k} C_{2,i+1,j,k-1}^n + D_{31,i,j+0.5,k} C_{2,i+1,j,k+1}^n}{\Delta x \Delta z} + \\ & + \frac{D_{32,i,j,k-0.5} C_{2,i,j-1,k-1}^n - D_{32,i,j,k-0.5} C_{2,i,j-1,k+1}^n - D_{32,i,j,k+0.5} C_{2,i,j+1,k-1}^n + D_{32,i,j,k+0.5} C_{2,i,j+1,k+1}^n}{\Delta y \Delta z} + \\ & + \frac{V_{1,i-0.5,j,k} C_{2,i-1,j,k}^n - V_{1,i+0.5,j,k} C_{2,i+1,j,k}^n}{2\Delta x} + \frac{V_{2,i,j-0.5,k} C_{2,i,j-1,k}^n - V_{2,i,j+0.5,k} C_{2,i,j+1,k}^n}{2\Delta y} + \\ & + \frac{V_{3,i,j,k-0.5} C_{2,i,j,k-1}^n - V_{3,i,j,k+0.5} C_{2,i,j,k+1}^n}{2\Delta z}, \end{aligned}$$

and after grouping this equation, we get:

$$\tilde{a}_{i,j,k} C_{2,i-1,j,k}^{n+1/3} - \tilde{b}_{i,j,k} C_{2,i,j,k}^{n+1/3} + \tilde{c}_{i,j,k} C_{2,i+1,j,k}^{n+1/3} = -\tilde{f}_{i,j,k}, \quad (71)$$

here : $\tilde{a}_{i,j,k} = \frac{D_{11,i-0.5,j,k}}{\Delta x^2}$,

$$\tilde{b}_{i,j,k} = \frac{m_g}{\Delta\tau/3} + \frac{(D_{11,i-0.5,j,k} + D_{11,i+0.5,j,k})}{\Delta x^2}, \quad \tilde{c}_{i,j,k} = \frac{D_{11,i+0.5,j,k}}{\Delta x^2},$$

$$\begin{aligned} \tilde{f}_{i,j,k} = & \frac{D_{12,i-0.5,j,k} C_{2,i-1,j-1,k}^{n+1/3} - D_{12,i-0.5,j,k} C_{2,i-1,j+1,k}^{n+1/3} - D_{12,i+0.5,j,k} C_{2,i+1,j-1,k}^{n+1/3} + D_{12,i+0.5,j,k} C_{2,i+1,j+1,k}^{n+1/3}}{\Delta x \Delta y} + \\ & + \frac{D_{13,i-0.5,j,k} C_{2,i-1,j,k-1}^{n+1/3} - D_{13,i-0.5,j,k} C_{2,i-1,j,k+1}^{n+1/3} - D_{13,i+0.5,j,k} C_{2,i+1,j,k-1}^{n+1/3} + D_{13,i+0.5,j,k} C_{2,i+1,j,k+1}^{n+1/3}}{\Delta x \Delta z} + \\ & + \frac{D_{22,i,j-0.5,k} C_{2,i,j-1,k}^n - (D_{22,i,j-0.5,k} + D_{22,i,j+0.5,k}) C_{2,i,j,k}^n + D_{22,i,j+0.5,k} C_{2,i,j+1,k}^n}{\Delta y^2} + \\ & + \frac{D_{21,i,j-0.5,k} C_{2,i-1,j-1,k}^n - D_{21,i,j-0.5,k} C_{2,i-1,j+1,k}^n - D_{21,i,j+0.5,k} C_{2,i+1,j-1,k}^n + D_{21,i,j+0.5,k} C_{2,i+1,j+1,k}^n}{\Delta x \Delta y} + \\ & + \frac{D_{23,i,j-0.5,k} C_{2,i,j-1,k-1}^n - D_{23,i,j-0.5,k} C_{2,i,j-1,k+1}^n - D_{23,i,j+0.5,k} C_{2,i,j+1,k-1}^n + D_{23,i,j+0.5,k} C_{2,i,j+1,k+1}^n}{\Delta y \Delta z} + \\ & + \frac{D_{33,i,j,k-0.5} C_{2,i,j,k-1}^n - (D_{33,i,j,k-0.5} + D_{33,i,j,k+0.5}) C_{2,i,j,k}^n + D_{33,i,j,k+0.5} C_{2,i,j,k+1}^n}{\Delta z^2} + \\ & + \frac{D_{31,i,j-0.5,k} C_{2,i-1,j,k-1}^n - D_{31,i,j-0.5,k} C_{2,i-1,j,k+1}^n - D_{31,i,j+0.5,k} C_{2,i+1,j,k-1}^n + D_{31,i,j+0.5,k} C_{2,i+1,j,k+1}^n}{\Delta x \Delta z} + \\ & + \frac{D_{32,i,j,k-0.5} C_{2,i,j-1,k-1}^n - D_{32,i,j,k-0.5} C_{2,i,j-1,k+1}^n - D_{32,i,j,k+0.5} C_{2,i,j+1,k-1}^n + D_{32,i,j,k+0.5} C_{2,i,j+1,k+1}^n}{\Delta y \Delta z} + \\ & + \frac{D_{33,i,j,k-0.5} C_{2,i,j,k-1}^n - (D_{33,i,j,k-0.5} + D_{33,i,j,k+0.5}) C_{2,i,j,k}^n + D_{33,i,j,k+0.5} C_{2,i,j,k+1}^n}{\Delta z^2} + \end{aligned}$$

$$\begin{aligned}
& + \frac{D_{31,i,j-0.5,k}C_{2,i-1,j,k-1}^n - D_{31,i,j-0.5,k}C_{2,i-1,j,k+1}^n - D_{31,i,j+0.5,k}C_{2,i+1,j,k-1}^n + D_{31,i,j+0.5,k}C_{2,i+1,j,k+1}^n}{\Delta x \Delta z} \\
& + \frac{D_{32,i,j,k-0.5}C_{2,i,j-1,k-1}^n - D_{32,i,j,k-0.5}C_{2,i,j-1,k+1}^n - D_{32,i,j,k+0.5}C_{2,i,j+1,k-1}^n + D_{32,i,j,k+0.5}C_{2,i,j+1,k+1}^n}{\Delta y \Delta z} \\
& + \frac{V_{1,i-0.5,j,k}C_{2,i-1,j,k}^n - V_{1,i+0.5,j,k}C_{2,i+1,j,k}^n}{2\Delta x} + \frac{V_{2,i,j-0.5,k}C_{2,i,j-1,k}^n - V_{2,i,j+0.5,k}C_{2,i,j+1,k}^n}{2\Delta y} \\
& + \frac{V_{3,i,j,k-0.5}C_{2,i,j,k-1}^n - V_{3,i,j,k+0.5}C_{2,i,j,k+1}^n}{2\Delta z} + \frac{m_g C_{2,i,j,k}^n}{\Delta \tau / 3}.
\end{aligned}$$

As above, we obtain follows from the approximation of (35) the boundary condition with respect to Ox :

$$\frac{-3C_{2,0,j,k}^{n+1/3} + 4C_{2,1,j,k}^{n+1/3} - C_{2,2,j,k}^{n+1/3}}{2\Delta x} = -\iota(C_{2,1,j,k} - C_2^0), \quad (72)$$

we find $C_{2,2,j,k}^{n+1/3}$ via the system of tridiagonal equations (65) at $i = 1$:

$$\begin{aligned}
& \tilde{a}_{1,j,k}C_{2,0,j,k}^{n+1/3} - \tilde{b}_{1,j,k}C_{2,1,j,k}^{n+1/3} + \tilde{c}_{1,j,k}C_{2,2,j,k}^{n+1/3} = -\tilde{f}_{1,j,k}, \\
& C_{2,2,j,k}^{n+1/3} = -\frac{\tilde{a}_{1,j,k}}{\tilde{c}_{1,j,k}}C_{2,0,j,k}^{n+1/3} + \frac{\tilde{b}_{1,j,k}}{\tilde{c}_{1,j,k}}C_{2,1,j,k}^{n+1/3} - \frac{\tilde{f}_{1,j,k}}{\tilde{c}_{1,j,k}},
\end{aligned} \quad (73)$$

we get $C_{2,0,j,k}^{n+1/3}$ by substituting $C_{2,2,j,k}^{n+1/3}$ in (66) into (65):

$$C_{2,0,j,k}^{n+1/3} = \frac{\tilde{b}_{1,j,k} - 4\tilde{c}_{1,j,k} - 2\iota\Delta x\tilde{c}_{1,j,k}}{\tilde{a}_{1,j,k} - 3\tilde{c}_{1,j,k}}C_{2,1,j,k}^{n+1/3} + \frac{2\iota\Delta x\tilde{c}_{1,j,k}C_2^0 - \tilde{f}_{1,j,k}}{\tilde{a}_{1,j,k} - 3\tilde{c}_{1,j,k}}.$$

Sweep method coefficients $\tilde{\alpha}_{0,j,k}$ and $\tilde{\beta}_{0,j,k}$ are calculated by the following formula:

$$\tilde{\alpha}_{0,j,k} = \frac{\tilde{b}_{1,j,k} - 4\tilde{c}_{1,j,k} - 2\iota\Delta x\tilde{c}_{1,j,k}}{\tilde{a}_{1,j,k} - 3\tilde{c}_{1,j,k}}, \quad \tilde{\beta}_{0,j,k} = \frac{2\iota\Delta x\tilde{c}_{1,j,k}C_2^0 - \tilde{f}_{1,j,k}}{\tilde{a}_{1,j,k} - 3\tilde{c}_{1,j,k}}.$$

As above, we obtain follows from the approximation of (36) the boundary condition with respect to Ox :

$$\frac{C_{2,N-2,j,k}^{n+1/3} - 4C_{2,N-1,j,k}^{n+1/3} + 3C_{2,N,j,k}^{n+1/3}}{2\Delta x} = -\iota(C_{2,N-1,j,k} - C_2^0). \quad (74)$$

Using sweep method, at $N, N-1$ and $N-2$, we find $C_{2,N-1,j,k}^{n+1/3}$ and $C_{2,N-2,j,k}^{n+1/3}$:

$$C_{2,N-1,j,k}^{n+1/3} = \tilde{\alpha}_{N-1,j,k}C_{1,N,j,k}^{n+1/3} + \tilde{\beta}_{N-1,j,k}, \quad (75)$$

$$\begin{aligned}
C_{2,N-2,j,k}^{n+1/3} &= \tilde{\alpha}_{N-2,j,k}C_{2,N-1,j,k}^{n+1/3} + \tilde{\beta}_{N-2,j,k} = \\
&= \tilde{\alpha}_{N-2,j,k}\tilde{\alpha}_{N-1,j,k}C_{2,N,j,k}^{n+1/3} + \tilde{\alpha}_{N-2,j,k}\tilde{\beta}_{N-1,j,k} + \tilde{\beta}_{N-2,j,k}.
\end{aligned} \quad (76)$$

We find $C_{2,N,j,k}^{n+1/3}$ by substituting $C_{2,N-1,j,k}^{n+1/3}$ in (68) and $C_{2,N-2,j,k}^{n+1/3}$ in (69) into (67):

$$C_{2,N,j,k}^{n+1/3} = \frac{4\tilde{\beta}_{N-1,j,k} - 2\iota\Delta x\tilde{\beta}_{N-1,j,k} + 2\iota\Delta xC_2^0 - \tilde{\alpha}_{N-2,j,k}\tilde{\beta}_{N-1,j,k} - \tilde{\beta}_{N-2,j,k}}{\tilde{\alpha}_{N-2,j,k}\tilde{\alpha}_{N-1,j,k} + 2\iota\Delta x\tilde{\alpha}_{N-1,j,k} - 4\tilde{\alpha}_{N-1,j,k} + 3}.$$

$C_{2,N-1,j,k}^{n+1/3}, C_{2,N-2,j,k}^{n+1/3}, \dots, C_{2,1,j,k}^{n+1/3}$ concentration values are connected to each others by following:

$$C_{2,i,j,k}^{n+1/3} = \tilde{\alpha}_{i,j,k}C_{2,i+1,j,k}^{n+1/3} + \tilde{\beta}_{i,j,k}, \quad i = \overline{N-1, 1}, \quad j = \overline{0, M}, \quad k = \overline{0, L}.$$

Thus, a mathematical model and a numerical solution algorithm were developed to study and predict the underground mining process, make the right decisions, and conduct computational experiments.

4 Analysis of results

The calculation results were performed using the Python programming language. When solving the problem, the dimensions of the sphere were taken as follows: $0 < x < 100(m)$, $0 < y < 50(m)$, z – varies depending on the ore reserve. Figures 1-10 show the distribution of acid on the ore-bearing plain within the mine.

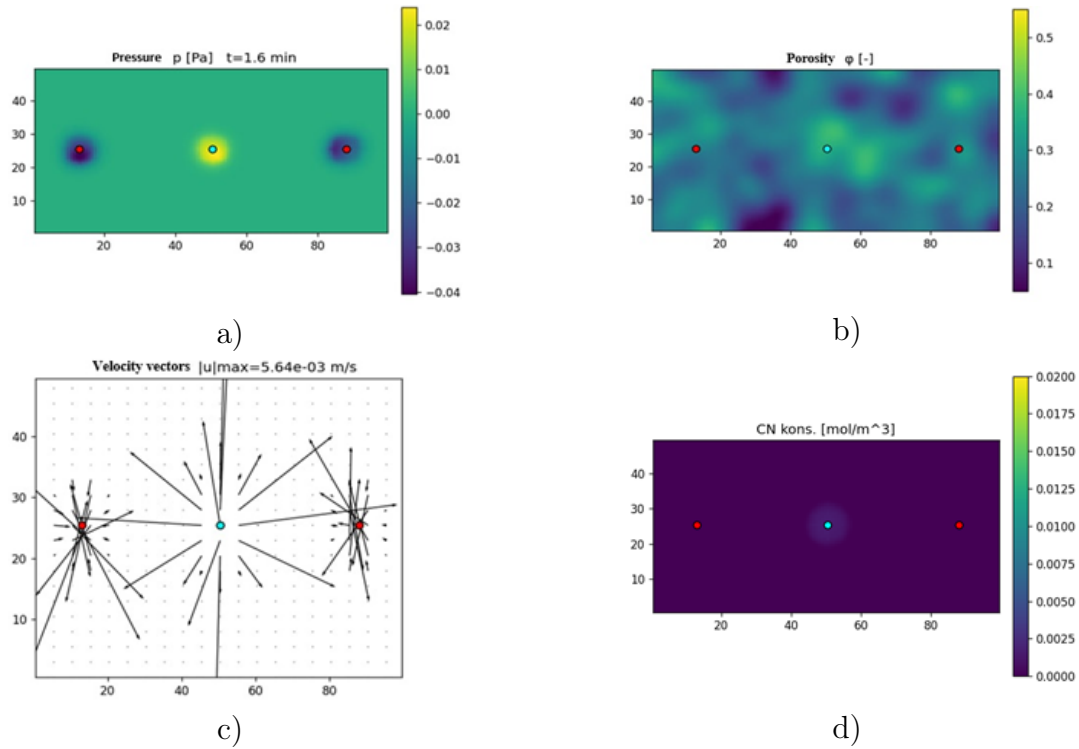


Figure 1 Pressure distribution in the area at $t = 1.6$ minutes (a), porosity (b), The velocity vectors (c) and concentration (d) changes are shown

From the initial calculation experiments that the velocity vectors are very large in the areas of high porosity of the field and exist only around the wells, in the rest of the field there is no movement. Fluid is supplied from the center and pumps are drawn from the production wells. It can be seen that the pressure distribution in the field is high around the injection well, low around the production wells and evenly distributed in the rest of the field. The porosity has not changed from the initial state and the velocity vectors are large precisely in areas with high porosity. The concentration of the injection well has changed slightly, in the rest of the places it is evenly distributed and has not reached the production wells.

In a porous medium, it can be seen that the pressure distribution around the injection well is significantly increased and the area of low pressure around the production wells is enlarged. The velocity vectors are slightly normalized. The porosity of the medium is almost static and changes very little. It was observed that the concentration slowly spread around the injection well.

At 12 minutes of time, it can be seen that the process has developed dramatically. The distribution of high pressure in the field is more than 10 m radius from the center and

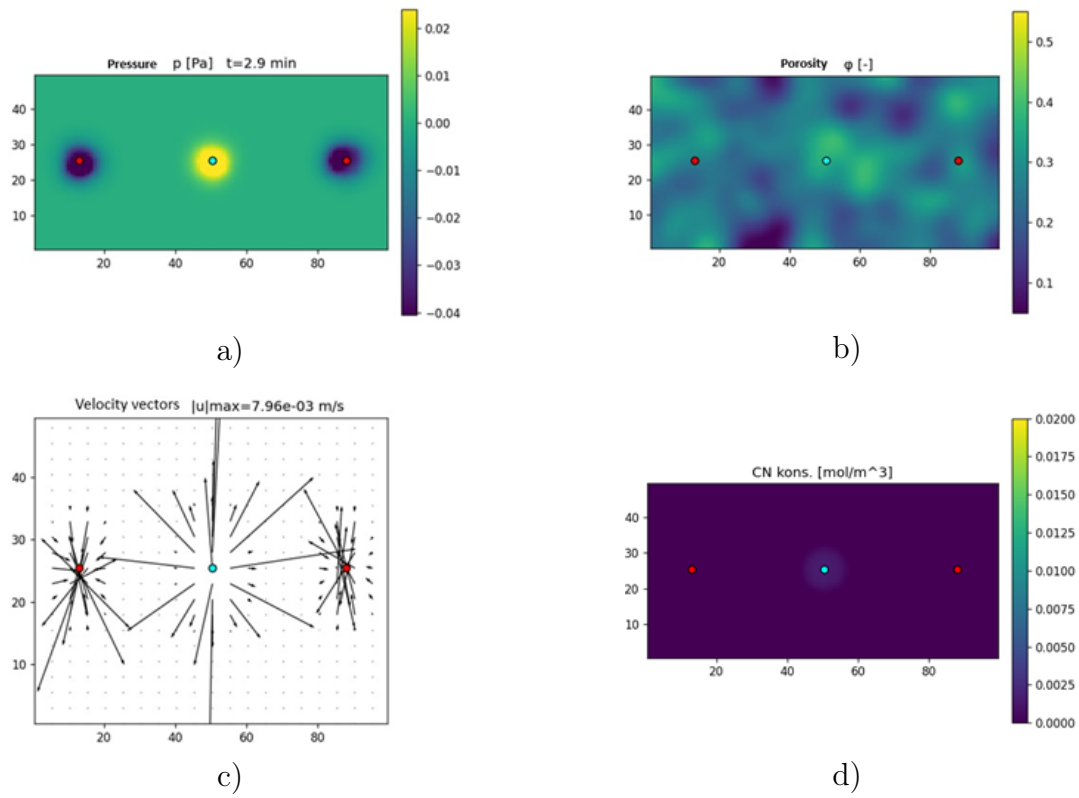


Figure 2 Pressure distribution in the area at $t = 2.9$ minutes (a), porosity (b), the velocity vectors (c) and concentration (d) changes are shown

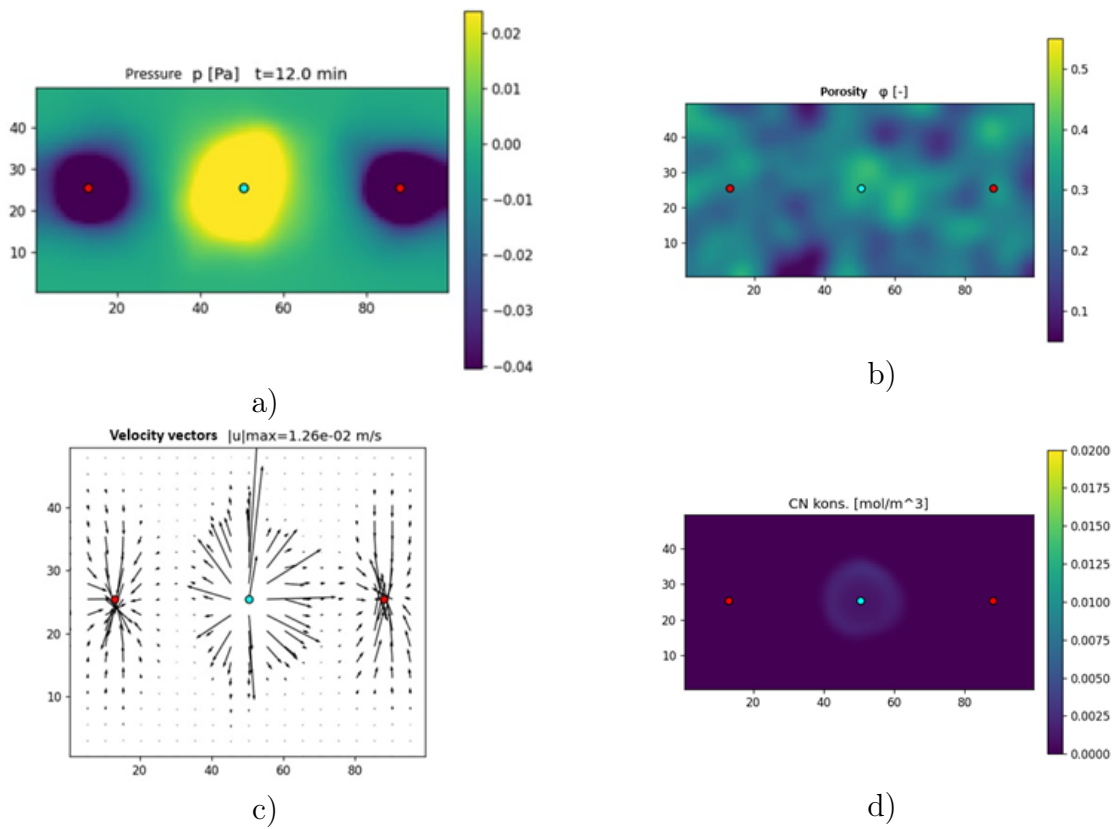


Figure 3 Pressure distribution in the area at $t = 12$ minutes (a), porosity (b), the velocity vectors (c) and concentration (d) changes are shown

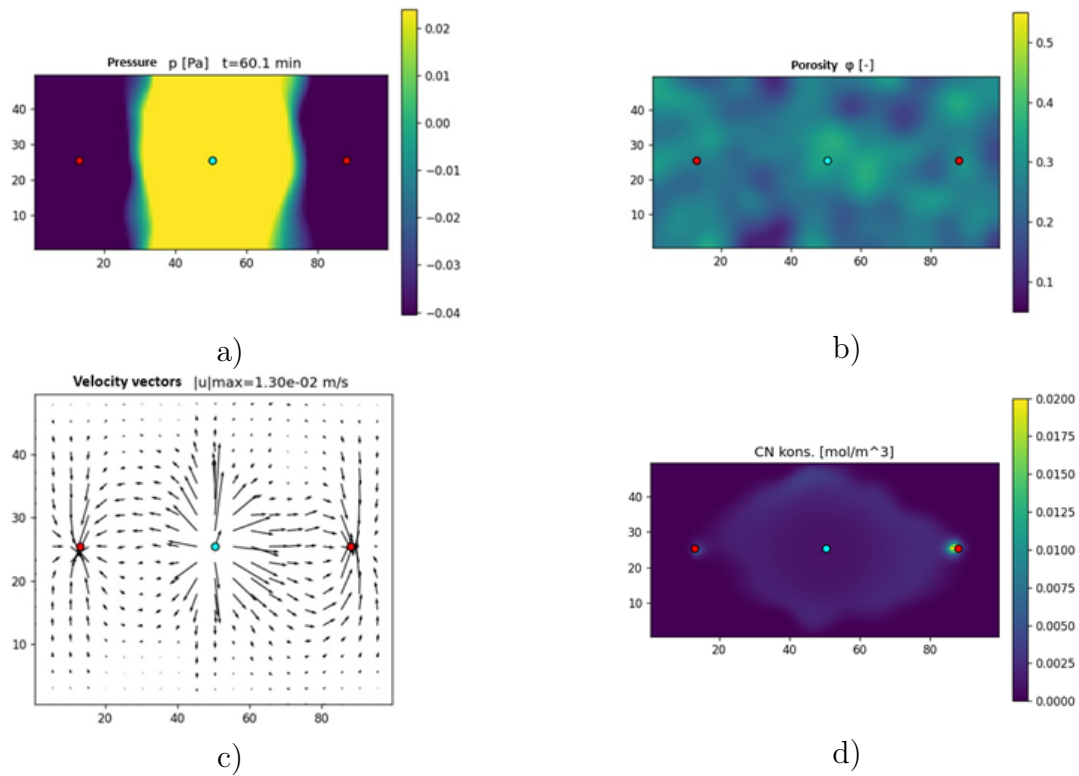


Figure 4 Pressure distribution in the area at $t = 1$ hour (a), porosity (b), The velocity vectors (c) and concentration (d) changes are shown

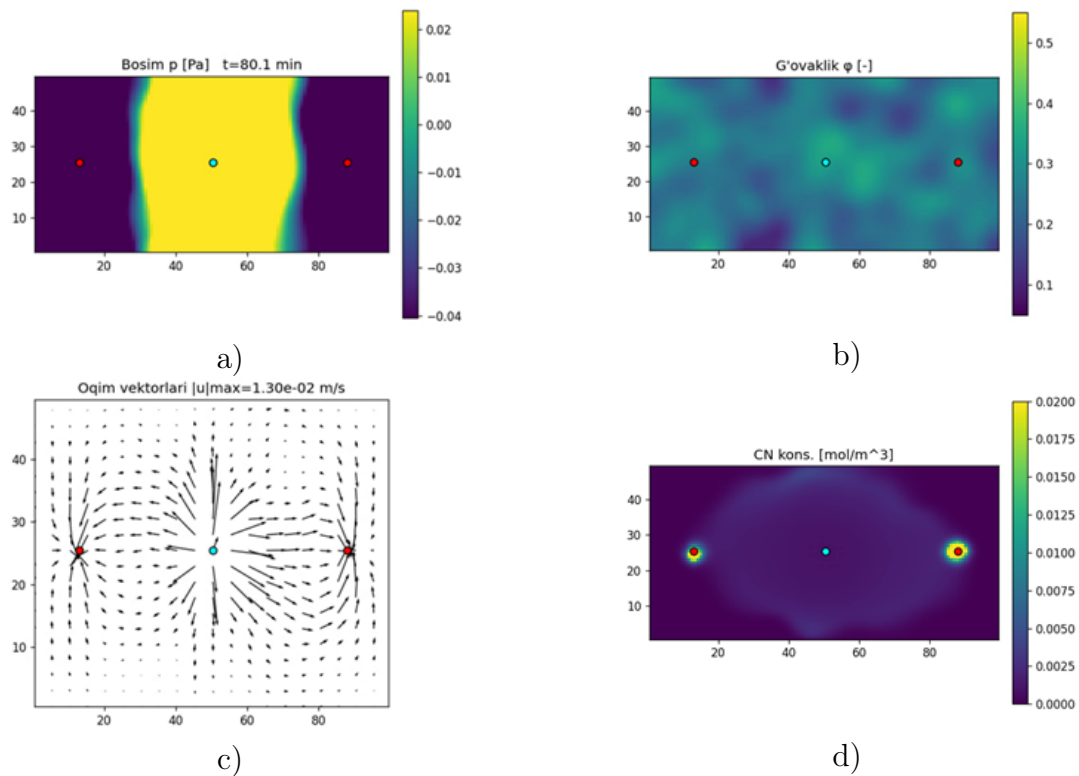


Figure 5 Pressure distribution in the area at $t = 1$ hour 20 minutes (a), porosity (b), The velocity vectors (c) and concentration (d) changes are shown

around the production wells low pressure expanded due to the operation of the pumps. The pressure in the production and injection wells are almost affected. Velocity vectors

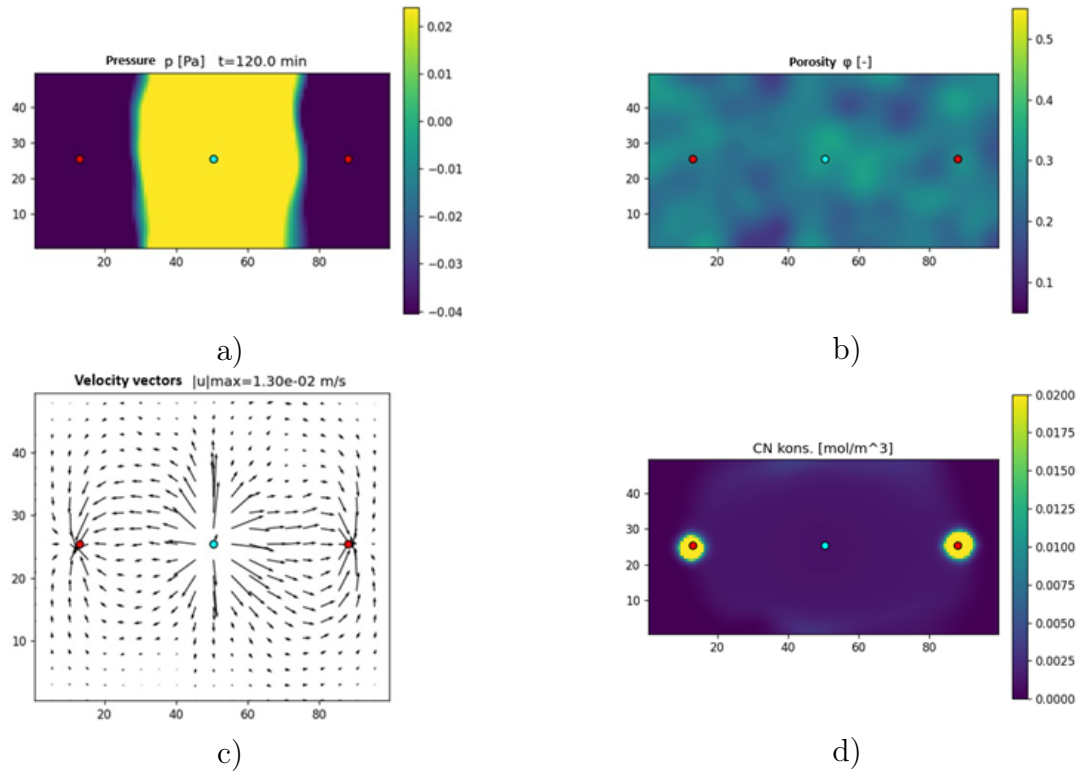


Figure 6 Pressure distribution in the area at $t = 2$ hours (a), porosity (b), The velocity vectors (c) and concentration (d) changes are shown

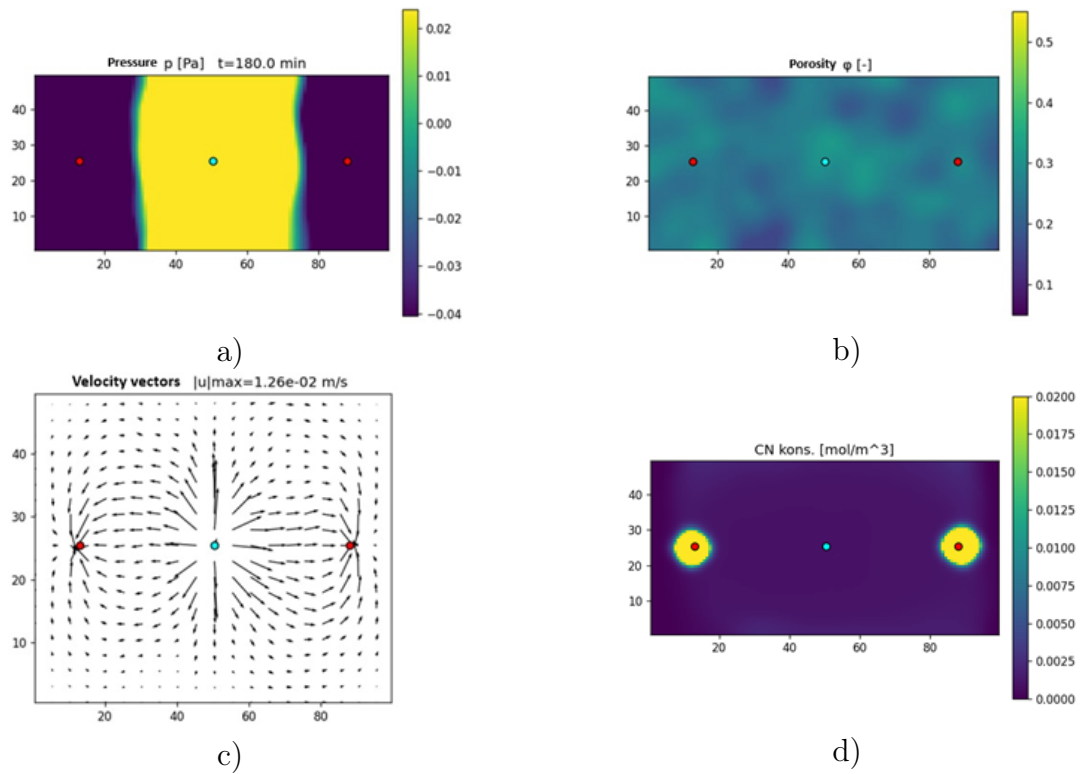


Figure 7 Pressure distribution in the area at $t = 3$ hours (a), porosity (b), The velocity vectors (c) and concentration (d) changes are shown

are much more stagnant and decelerated due to changes in porosity. It can be seen that the concentration has shifted significantly.

It can be seen that the pressures of the injection well and production wells have reached a state of complete equilibrium. It can be seen that the porosity has increased almost everywhere in the field and the permeability has increased, shifting from anisotropic to isotropic, as a result of which the velocity vectors of the flow have reached a nearly stationary state. It is observed that the concentration has reached the production well and increases around the production wells.

In the field, the pressures of production wells and injection wells are full balanced. The change of porosity and velocity vectors is almost unchanged from 20 minutes ago. And the concentration increased significantly around the production wells.

The pressures of the field have reached a state of complete balance. Porosity and velocity vectors are almost stationary. And the concentration increased and accumulated around the production well.

It can be seen that the situation at 3 hours after the start of the process is almost the same as at 2 hours. The porosity is very close to a homogeneous state and the velocity vectors are evenly distributed throughout the field, i.e. there is a flow throughout the entire field. The concentration is sufficient around the production well, i.e. the mixture is sufficiently saturated, which means that it is easier to pump the mixture.

5 Conclusion

This study presented a comprehensive mathematical model, numerical solution algorithm, and software to analyze the hydrodynamic processes involved in ISL in three-dimensional porous media. The rate of change of these hydrodynamic parameters depends on the pressure; showing exponential behavior under high pressure and linear behavior under low pressure conditions.

By incorporating filtration, diffusion, and kinetic factors, the model provides a deeper understanding of how pressure variations, permeability, and porosity affect the extraction process. The use of numerical methods to solve complex parabolic-type quasi-linear eigenvalue equations is shown to be effective in simulating real-world ISL processes. The rate of change of these hydrodynamic parameters is pressure-dependent; exhibiting exponential behavior at high pressure and linear behavior at low pressure. It should be noted that in the process of ISL, a chemical reaction occurs as a result of the reagent's effect on ore deposits, and the substance passes from one phase to another, as a result of which the hydrodynamic parameters of the pore medium (filtration and porosity coefficients) and the pressure in the ore reservoir change.

The main result of this study is the significant effect of pressure variation on hydrodynamic parameters, especially on injection and extraction of rhythm. These changes directly affect the efficiency of mineral processing and possible ecological consequences such as groundwater contamination. The proposed mathematical model, numerical solution algorithm, and software allow for improved monitoring, prediction, and optimization of ISL operations that are both economically feasible and ecologically safe.

Future research will focus on refining this model to include dynamic factors such as chemical interactions, multiphase flow motion, and integration of real-time field data. Further advances in computational algorithms and software will also increase the accuracy and applicability of simulations, leading to more sustainable and efficient mining practices.

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УДК 519.6+51-74::628.395

ТРЁХМЕРНАЯ МАТЕМАТИЧЕСКАЯ МОДЕЛЬ И АЛГОРИТМ ЧИСЛЕННОГО РЕШЕНИЯ ДЛЯ МОНИТОРИНГА И ПРОГНОЗИРОВАНИЯ ПРОЦЕССОВ ПОДЗЕМНОГО ВЫЩЕЛАЧИВАНИЯ В ПОРИСТОЙ СРЕДЕ

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В статье анализируются гидродинамические процессы, связанные с подземной добычей полезных ископаемых, в частности, с кислотной экстракцией драгоценных металлов из рудных месторождений. Для комплексного изучения, мониторинга и прогнозирования поведения объекта разработана математическая модель (ММ), основанная на фильтрационно-конвективных и диффузионных процессах, характерных для фильтрации подземных флюидов. Эта модель учитывает влияние различных гидродинамических параметров, в частности, коэффициента фильтрации и средней пористости, которые являются функциями уровня давления и кинетики процесса. Анализ постановки задачи показывает, что изменение давления в рудной залежи в результате заливки и извлечения раствора напрямую влияет на коэффициенты проницаемости и пористости пласта. Результаты экспериментов показали, что изменение гидродинамических параметров пропорционально изменению давления, при этом наблюдается экспоненциальная зависимость при высоком давлении и линейная зависимость при низком давлении. Следует отметить, что в процессе подземного выщелачивания (ПВ) в результате воздействия реагента на рудные залежи происходила химическая реакция и вещество переходило из одной фазы в другую, в результате чего наблюдались изменения гидродинамических параметров поровой среды (коэффициентов фильтрации и пористости) и давления в рудном пласте.

Ключевые слова: подземное выщелачивание, математическое моделирование, численный алгоритм, минералы, фильтрация и диффузия жидкостей, кинетика процесса.

Цитирование: *Равшанов Н., Усмонов Л.С.* Трёхмерная математическая модель и алгоритм численного решения для мониторинга и прогнозирования процессов подземного выщелачивания в пористой среде // Проблемы вычислительной и прикладной математики. – 2025. – № 6(70). – С. 26-47.

DOI: https://doi.org/10.71310/pcam.6_70.2025.03

ПРОБЛЕМЫ ВЫЧИСЛИТЕЛЬНОЙ И ПРИКЛАДНОЙ МАТЕМАТИКИ

№ 6(70) 2025

Журнал основан в 2015 году.

Издается 6 раз в год.

Учредитель:

Научно-исследовательский институт развития цифровых технологий и
искусственного интеллекта.

Главный редактор:

Равшанов Н.

Заместители главного редактора:

Арипов М.М., Шадиметов Х.М., Ахмедов Д.Д.

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Журнал зарегистрирован в Агентстве информации и массовых коммуникаций при
Администрации Президента Республики Узбекистан.

Регистрационное свидетельство №0856 от 5 августа 2015 года.

ISSN 2181-8460, eISSN 2181-046X

При перепечатке материалов ссылка на журнал обязательна.

За точность фактов и достоверность информации ответственность несут авторы.

Адрес редакции:

100125, г. Ташкент, м-в. Буз-2, 17А.

Тел.: +(998) 712-319-253, 712-319-249.

Э-почта: journals@airi.uz.

Веб-сайт: <https://journals.airi.uz>.

Дизайн и вёрстка:

Шарипов Х.Д.

Отпечатано в типографии НИИ РЦТИИ.

Подписано в печать 25.12.2025 г.

Формат 60x84 1/8. Заказ №8. Тираж 100 экз.

PROBLEMS OF COMPUTATIONAL AND APPLIED MATHEMATICS

No. 6(70) 2025

The journal was established in 2015.
6 issues are published per year.

Founder:

Digital Technologies and Artificial Intelligence Development Research Institute.

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Korea).

The journal is registered by Agency of Information and Mass Communications under the
Administration of the President of the Republic of Uzbekistan.

The registration certificate No. 0856 of 5 August 2015.

ISSN 2181-8460, eISSN 2181-046X

At a reprint of materials the reference to the journal is obligatory.

Authors are responsible for the accuracy of the facts and reliability of the information.

Address:

100125, Tashkent, Buz-2, 17A.

Tel.: +(998) 712-319-253, 712-319-249.

E-mail: journals@airi.uz.

Web-site: <https://journals.airi.uz>.

Layout design:

Sharipov Kh.D.

DTAIDRI printing office.

Signed for print 25.12.2025

Format 60x84 1/8. Order No. 8. Print run of 100 copies.

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