Numerical Solution of Rare Metal Leaching Problem

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Abstract

It is well known that a lot of chemical and physical processes take place on the surfaces of interaction between solid and liquid substances. These processes include a very important technological process of uranium, nickel, copper, precious metal and other solid compound extraction - in-situ leaching. In this article we will rely on the mathematical description of these complex systems proposed by A.M. Meirmanov, where the main idea is the presence of new conditions on a free (unknown) boundary between liquid and solid phases ("pore space - solid skeleton"). These conditions express the usual laws of mass conservation of mass and the development of the mathematical model describing the processes at the macroscopic level. The method proposed in the book allows us to study numerically the dependence ways of free boundary dynamics on a heterogeneous solution distribution velocity and external parameters (reagent temperature, pressure and concentration).

Keywords: solid-liquid environment interface, free-boundary problem, fluid dynamics.

1. Introduction

This article uses the results of [1], [2], where they presented the microscopic model of free boundary motion and its numerical solution for one-dimensional geometry of the pore space was presented. Unfortunately, it was not possible to record the fluctuation of the acid concentration values on the free boundary in [2]. Therefore, in this work, they decided to start with a microscopic model and complete it with new numerical simulations, where the acid concentration fluctuations at the free boundary will be shown clearly. The most important part of the work is the numerical solution of the macroscopic (averaged) model obtained using the methods developed in [3]. In particular, completely new transfer equations are derived for chemical reaction products that take into account the boundary conditions on the free boundary at the microscopic level. Here, they use some heuristic axioms, which can be proved if necessary, and to preserve accuracy, they use the equivalent form of differential equations as a system of integral identities. Of course, the derivation of a microscopic model should be based on classical mechanics equations (see, for example, [4]). However, the use of engineering methods in homogenization (as in [4]) can lead to errors. For example, the authors of [4] did not understand that a microscopic model is the problem with a free boundary, which turns into a system of differential equations with unknown coefficients at a macroscopic level. These factors can only be determined only by the microstructure consideration.

2.Methods

The article discusses the physical processes in a limited area Ω from $\mathbb{R}^3$. A part of S^+ of boundary S from the region Ω models injection wells, a part of S^- models the pumping wells, and S^0

models an impenetrable boundary Ω. In addition, the region Ω consists of the region $\Omega_f(t)$ - the pore space, the region $\Omega_s(t)$ - an absolutely solid soil skeleton, and a free border $\Gamma(t)$ (see Fig. 1). Such tasks are called free boundary problems.
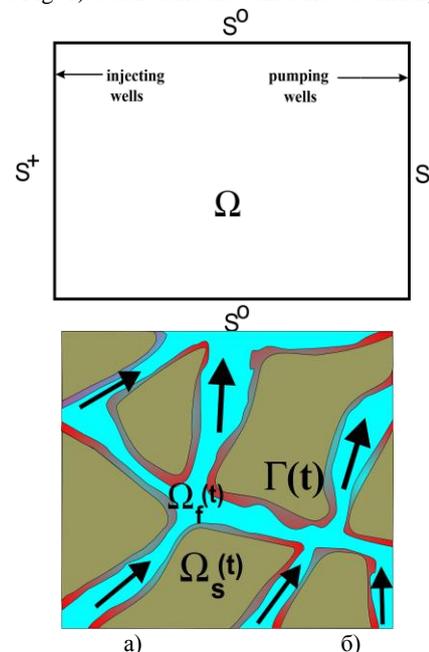

Figure 1 – a) underground leaching model, б) pore space structure

In presented study, they use the conventional equations of continuum mechanics [5] and the well-known chemical laws [6], [7] at the microscopic level.
Let's use the Stokes system of equations for an incompressible

viscous fluid to simulate the dynamics of fluid in the pores at the microscopic level. Such an approximation is quite acceptable. In fact, the movement of fluid in the pores occurs very slowly (about 5–8 meters per year), and the convection terms in the Navier – Stokes equations can be neglected.

There are many different scenarios for the distribution of impurities in the pore space at the microscopic level, where convection and diffusion should be taken into account. In accordance with the general theory of differential equations, it is necessary to know the boundary condition for the impurity at the outer boundary S (Fig. 1). Such a boundary condition is quite acceptable For the concentration of acid. Besides, a reverse flow is formed from the free boundary $\Gamma(t)$ inside the pore space. This flow prevents the penetration of acid to the solid skeleton. The lack of diffusion implies the absence of chemical reactions at the border $\Gamma(t)$. Thus, the diffusion-convection equation is the main description of the acid component.

Any boundary condition on S^- for the concentration of chemical reaction products does not make sense, since it is impossible to predict how many reaction products will appear in a pump well. Therefore, the transfer equation is used for the concentrations of chemical reaction products. The transfer equation is the first order equation which requires a boundary condition only on the part of the boundary $\partial\Omega_f(t)$ where the fluid flows into the pore space. The free boundary $\Gamma(t)$ and injection wells S^+ are the part of the boundary $\partial\Omega_f(t)$ where we know the exact concentration of chemical reaction products.
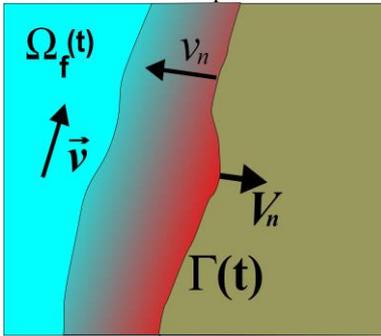

Figure 2 – Diffusion and convection near the free boundary

Let's note that the process of fluid diffusion is very slow and comparable with convection by speed. Therefore, it can create some fluctuations in the reagent concentration at the free boundary and, consequently, the fluctuations of chemical reaction product concentration in pumping wells. In fact, the flow rate of fluid from the free border is proportional to the concentration of acid and increases with its increase. The predominance of fluid outflow from the free boundary reduces the diffusion of the reagent and leads to the solution concentration decrease on the free boundary $\Gamma(t)$. In its turn, this means the decrease of fluid outflow from the free boundary and the predominance of acid diffusion from the free boundary inward. An increase of reagent diffusion with respect to the free boundary leads to the reagent concentration increase at the free boundary, etc. (see Fig. 2).

3.Main part

For the case of a single spatial variable (Fig. 3), the problem of diffusional propagation of a mixture for an incompressible fluid within the region $0 < x < X(t)$ at $t > 0$ will be the following

$$\frac{\partial p}{\partial x} = 0, \tag{1}$$

$$\frac{\partial v}{\partial x} = 0, \tag{2}$$

$$\frac{\partial c}{\partial t} + v\frac{\partial c}{\partial x} = \alpha_c\frac{\partial^2 c}{\partial x^2}, \tag{3}$$

and supplemented by initial conditions

$$p(0,t) = p^+(t), \quad c(0,t) = c^+(t), \quad t > 0, \tag{4}$$

$$X(0) = X_0, \quad c(x,0) = c_0(x), \quad 0 < x < X_0. \tag{5}$$

and boundary conditions at $\Gamma(t)$

$$\left(\frac{dX}{dt} + \beta - v\right)c + \alpha_c\frac{\partial c}{\partial x} = 0, \quad x = X(t), \, t > 0, \tag{6}$$

$$v(t) = -\frac{dX}{dt}(t)\frac{(\rho_s - \rho_f)}{\rho_f}, \quad t > 0, \tag{7}$$

$$\frac{dX}{dt} = \beta\,\gamma\,c, \quad x = X(t), \, t > 0, \tag{8}$$

where $\frac{dX}{dt}$ – the velocity of $\Gamma(t)$, $v(t)$ – standard fluid velocity, $p(0,t)$ – fluid pressure, c – reagent concentration, ρ_s and ρ_f – dimensionless densities of solid skeleton and pore fluid, correlated to the average density of water ρ^0, β and γ are some nonnegative constants.
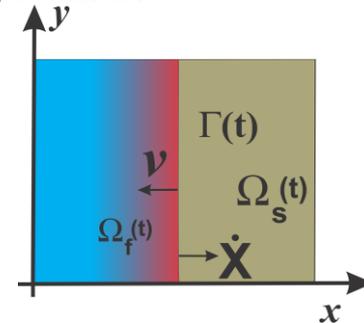

Figure 3 – One dimensional movement

The numerical methods for the solution of (3) are well developed now. These are such methods such as the finite difference method, the finite element method, the line method, etc. Finite-difference methods for one-dimensional convection-diffusion equation solution can be considered in accordance with the number of involved spatial points of the computational grid and the number of time levels in use.

It is sufficient to use the finite difference method for a one-dimensional problem. This approach begins with domain discretization by the variables x and t.

Let's divide the segment $[0,1]$ into M subintervals so that $Mh = 1$ and the interval $[0,T]$ into N subintervals, such

that $Nl = T$. After this we approximate $c(x,t)$ as c_i^n.

Thus, the points of the grid (x_i, t_n) are determined by the following formula:

$$x_i = i\,h, \quad 0,1,2,\ldots,M, \tag{9}$$

$$t_n = n\,l, \quad 0,1,2,\ldots,N, \tag{10}$$

where M and N are constants.

This explicit method uses the following approximations for $\partial c/\partial t$, $\partial c/\partial x$ and $\partial^2 c/\partial x^2$

$$\frac{\partial c}{\partial t} \simeq \frac{c_i^{n+1}-c_i^n}{\Delta t}, \quad \frac{\partial c}{\partial x} \simeq \frac{c_{i+1}^n-c_{i-1}^n}{2h}, \quad \frac{\partial^2 c}{\partial x^2} \simeq \frac{c_{i-1}^n-2c_i^n+c_{i+1}^n}{h^2}, \tag{11}$$

where $\Delta t = t^n - t^{n-1}$ and h is a uniform grid interval (grid spacing).

The introduction of the abovementioned approximations in (3) gives the following equation of finite differences:

$$c_i^{n+1} = c_i^n + a\left(c_{i-1}^n - 2c_i^n + c_{i+1}^n\right) - b\,v_i^{n+1}\left(c_{i+1}^n - c_{i-1}^n\right), \tag{12}$$

where $a = \alpha_c\,\Delta t/h^2$, $b = \Delta t/2h$ are the stability criteria.

$$h < \frac{2\,\alpha_c}{v_i^{n+1}}, \quad \Delta t < \frac{h^2}{2\,\alpha_c}. \tag{13}$$

One should determine (7) here:

$$v_i^{n+1} = -\beta\,\gamma\,c_i^n\left(\frac{\rho_s-\rho_f}{\rho_f}\right). \tag{14}$$

And finally, let's determine the condition for a free boundary in the following form:

$$c_i^{n+1} = -\frac{1}{\beta\,\gamma}\left(v_i^{n+1} - \beta - \frac{\alpha_c}{h}(1 - c_{i-1}^{n+1})\right). \tag{15}$$

Let determine the position of the free boundary and the concentration of the reagent on it for $\gamma = 1$, $D = 2822\frac{\mu m^2}{sec}$, $L = 16\mu m$, $T = 1sec$ and different values of c^+ (see fig. 4-5).
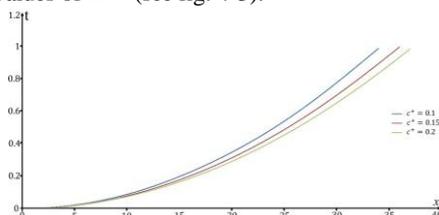

Figure 4 – The position of the free boundary at various values of c^+
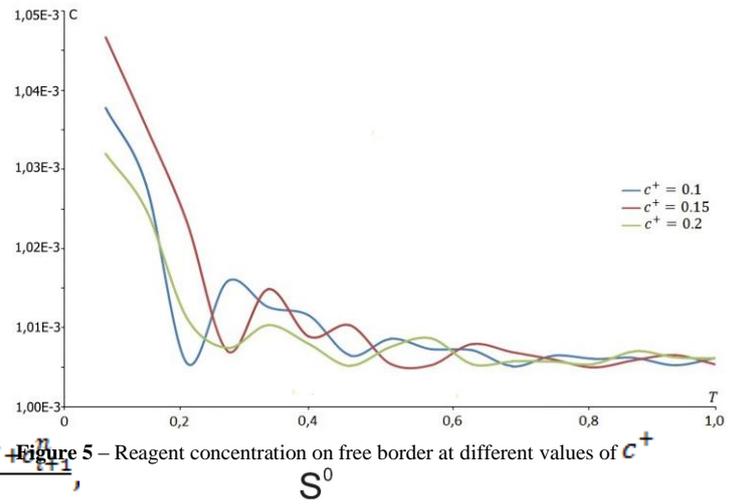

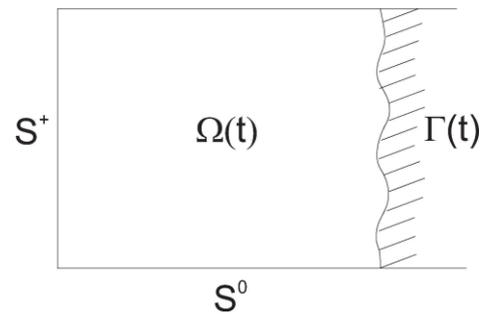**Figure 5** – Reagent concentration on free border at different values of c^+

Figure 6 – Two-dimensional area

In the case of two spatial variables, the system of differential equations in the region $\Omega = \{0 < x_1 < L, 0 < x_2 < H\}$ (see Fig. 6) for fluid velocity v, fluid pressure p and reagent concentration c has the following form:

$$\alpha_\mu\,\Delta v - \nabla p = 0, \tag{16}$$

$$\nabla \cdot v = 0, \tag{17}$$

$$\frac{\partial c}{\partial t} + v \cdot \nabla c = \alpha_c\,\Delta c \tag{18}$$

and supplemented by the following boundary conditions:

$$(d_n + \beta - v_n)\,c + \alpha_c\frac{\partial c}{\partial n} = 0, \tag{19}$$

$$v_n = -d_n\,\delta, \tag{20}$$

$$v - v_n \cdot n = 0, \tag{21}$$

$$d_n = \beta\,\gamma\,c, \tag{22}$$

on the free boundary $\Gamma(t)$ at $t > 0$, where d_n – the velocity of the boundary $\Gamma(t)$ in the direction of the external normal n with respect to the region $\Omega_f(t)$, v_n – the normal velocity of the fluid, $\alpha_\mu = \frac{\mu}{TLg\rho^0}$, $\alpha_c = \frac{DT}{L^2}$, μ – the velocity of the fluid in the pores, L – the characteristic size of the considered

region, T – the characteristic time of the process, g – gravity force, D – diffusion ratio.

The following condition is performed on the boundary S^+:

$$(2\,\alpha_\mu\,\mathbb{D}(v) - p\,\mathbb{I})\cdot n = -p^+ n \tag{23}$$

And

$$c = c^+. \tag{24}$$

At the boundary S^0 which is impermeable for fluid:

$$v = 0 \tag{25}$$

and

$$\frac{\partial c}{\partial n} = 0. \tag{26}$$

The task is closed with initial conditions:

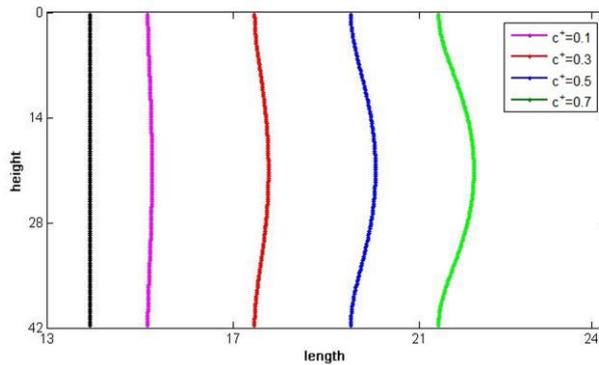$$\Gamma(0) = \Gamma_0,\ c(x,y,0) = c_0(x,y),\ (x,y) \in \Omega_0. \tag{27}$$

Figure 7 – The position of the free boundary at various values of c^+.

To calcualate a two-dimensional problem, we use the most popular of finite difference and MAC method [8], combining them with PISO method, which includes one prediction step and two correction steps. First of all, let's rewrite the system of equations (16) - (18) by coordinates. Let $v = (u, v)$.

$$\alpha_\mu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) - \frac{\partial p}{\partial x} = 0, \tag{28}$$

$$\alpha_\mu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) - \frac{\partial p}{\partial y} = 0, \tag{29}$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \tag{30}$$

$$\frac{\partial c}{\partial t} - \alpha_c \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right) + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} = 0 \tag{31}$$

As they described above, we will use two-dimensional homogeneous grids. The standard central-difference discretization Δ and ∇ at the vertices of a homogeneous grid will not give a stable discretization of Stokes equations. So the idea of MAC

method is to put the unknown $(u; v; p)$ in different places. In particular, the pressure p is located in the center of each cell, x-component of the velocity u is in the center of cell vertical edges, and y-component of the velocity v is in center of the horizontal edges.

Using the index system, where i is the column index, and j is the line index, the scheme MAC for (28) - (31) can be written as follows:

$$u_{i,j}^n = \left(u_{i-1,j}^n + u_{i+1,j}^n + u_{i,j-1}^n + u_{i,j+1}^n - h(p_{i,j}^n - p_{i-1,j}^n)\right)/4,$$

$$v_{i,j}^n = \left(v_{i-1,j}^n + v_{i+1,j}^n + v_{i,j-1}^n + v_{i,j+1}^n - h(p_{i,j-1}^n - p_{i,j}^n)\right)/4, \tag{33}$$

$$\frac{u_{i+1,j}^n - u_{i,j}^n}{h} + \frac{v_{i,j}^n - v_{i,j+1}^n}{h} = 0, \tag{34}$$

$$c_{i,j}^{n+1} = \alpha_c \Delta t \left(\frac{c_{i+1,j}^n - 2c_{i,j}^n + c_{i-1,j}^n}{h^2} + \frac{c_{i,j+1}^n - 2c_{i,j}^n + c_{i,j-1}^n}{h^2}\right) - \Delta t \left(u_{i,j}^n \frac{c_{i,j}^n - c_{i-1,j}^n}{h} - v_{i,j}^n \frac{c_{i,j-1}^n - c_{i,j}^n}{h}\right)$$

where n is the time layer.
Similarly, we can put down the condition for the free boundary (19) by coordinates.
Using numerical methods, they calculated the position of the free boundary for $D = 2822 \frac{\mu m^2}{sec}$, $L = 22\mu m$, $H = 8\mu m$, $T = 0.01 sec$, $\Gamma_0 = 14\mu m$, $c_0 = 0, p^+ = 1000, \gamma = 1$, and various values c^+ (see Fig. 7).

4.Summary

Thus, after the numerical experiments simulating the process of underground leaching of rare metals, they determined the fluctuations of chemical reaction product concentration values in a pump well.

5.Conclusions

In this article they studied new mathematical models describing the interaction of pore acid, filled with liquid, and the components that form the rock matrix [9], [10], [11]. Our approach was based on a detailed examination of the fundamental laws of mechanics and chemistry using a pore scale. Thus, the mathematical model obtained in pore scale cannot be used in practice, but its simple and mathematically correct form allows to perform further approximation by the system of homogeneous equations. Some numerical simulations show the distinctive features of the model. For example, at the microscopic level, monotonically increasing values β at a fixed concentration of c^+ on the free border and monotonously increasing concentration c^+ do not mean a monotonic behavior of the reagent concentration at the free border. On the other hand, the speed of the free boundary distribution is a monotonically increasing function of the constant β and c^+.

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