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Numerical implementation of the one-dimensional microscopic model of in-situ leaching

This publication is devoted to the numerical implementation of the mathematical model on a microscopic level of in-situ leaching process in the case of one space variable. The mathematical model is based on the common system of differential equations, when the fluid dynamics is described by the equation of motion of an incompressible fluid filling the pores of absolute solid ground skeleton, and dynamics of the active solution is described by the equation of diffusion-convection with point boundary conditions on the unknown free boundary between the fluid and the solid skeleton, expressing the conservation law of reagents. Numerical simulation by finite difference method is applied for the numerical solution of the problem. The nonlinear boundary conditions defined on the unknown free boundary is numerically solved by the iterative Newton's method. For a more precise description of the movement of the free boundary, interpolation method is detailed. The significance of computer modelling of in-situ leaching process on a micro scales is an ability to study the basic mechanisms of the flow of physical and chemical process comprises reacting an active solutions with a solid skeleton and its movement through the capillary. The article presents the results of the problem in the case of one space variable in the form of graphs, obtained in mathematical environment Matlab.
Key words: leaching, free boundary, microscopic model, numerical implementation.

Жумали А.С.

Численная реализация одномерной микроскопической модели подземного выщелачивания

Предлагаемая публикация посвящена численной реализации математической модели на микроскопическом уровне процесса подземного выщелачивания в случае одной пространственной переменной. Математическая модель основывается на общепринятой системе дифференциальных уравнений, когда динамика жидкости описывается уравнением движения несжимаемой жидкости, заполняющей поры абсолютно твердого скелета грунта, а динамика активной примеси описывается уравнением диффузии-конвекции с точечными краевыми условиями на неизвестной свободной границе между жидкостью и твердым скелетом, выражающими закон сохранения количества реагентов. Для численного решения поставленной задачи применялось численное моделирование методом конечных разностей. Нелинейное граничное условие, заданное на неизвестной свободной границе, численно решается итерационным методом Ньютона. Для более точного описания движения свободной границы детализируется метод интерполяции. Значимость компьютерного моделирования процесса подземного выщелачивания на микро масштабах заключается в возможности исследования основных механизмов протекания физико-химического процесса, заключающегося во взаимодействии активной примеси с твердым скелетом и ее движения по капилляру. В статье представлены результаты численного решения задачи в случае одной пространственной переменной в виде графиков, полученных в математической среде Matlab.
Ключевые слова: выщелачивание, свободная граница, микроскопическая модель, численная реализация.

Жұмәлі А.С.

Жерасты ерітінділеудің бір өлшемді микроскопиялық моделін сандық жүзеге асыру

Ұсынылып отырған басылымда бір кеңістіктік айнымалы жағдайындағы жерасты ерітінділеу үрдісінің микроскопиялық деңгейдегі бір өлшемді математикалық моделін сандық жүзеге асыру сипатталған. Математикалық модель жалпыға мәлім дифференциалдық теңдеулер жүйесіне негізделеді, яғни сұйық динамикасы жер қыртысының абсолют қатты скелетінің кеуектерін толтыратын сығылмайтын сұйық қозғаласы теңдеуімен сипатталады, ал белсенді қоспа динамикасы, реагенттер мөлшерінің сақталуы заңын өрнектейтін, сұйықтық пен қатты скелет арасындағы белгісіз еркін шекараға қойылған нақты шекаралық шарттары бар диффузия-конвекция теңдеуімен сипатталады. Қойылған есепті сандық түрде шешу үшін ақырлы айырымдар әдісімен сандық моделдеу қолданылды. Белгісіз еркін шекараға қойылған сызықсыз шекаралық шарт итерациялық Ньютон әдісімен сандық түрде шешіледі. Еркін шекара қозғалысын дәлірек сипаттау мақсатында интерполяция әдісі талданады. Жерасты ерітінділеу үрдісін микро масштабтарда компьютерлік моделдеудің маңыздылығы белсенді қоспаның қатты скелетпен байланысқа түсуіне негізделген физикалық, химиялық үрдістің негізгі ерекшеліктері мен оның капиллярдағы қозғалысын зерттеу мүмкіндігіне негізделеді. Мақалада бір өлшемді есептің сандық шешімінің нәтижелері Matlab математикалық ортасында алынған графиктер түрінде келтірілген.

Түйін сөздер: ерітінділеу, еркін шекара, микроскопиялық модель, сандық жүзеге асыру.

1 Introduction

The process of in-situ leaching is an environmentally friendly method of mining minerals such as uranium, copper, nickel, gold, etc. It is held by filing the active solution into a porous ground wherein the solution reacts with the solid material. The resulting product of the chemical interaction enters the liquid. This physical process is considered in a bounded domain Ω . The area Ω consists of the area Ω_f modeling the pore space, the area Ω_s simulating a solid skeleton and the boundary $X(t)$ between the pore space and solid skeleton (see fig. 1). The boundary $X(t)$ is unknown, because in the process of leaching the part of the soil dissolves and the soil is deformed over time. Such boundary is called free boundary and such problems are called free boundary problems.

Currently the leaching of rocks describes by the large range of mathematical models describing the physical processes at the macroscopic level (see [1] - [6] and references there in). In these models at each point of a continuous medium there are the solid skeleton and the liquid in pores. R. Burridge and J. B. Keller [7] and E. Sanchez-Palencia [8] were the first to state explicitly that mathematical models for filtration and seismic must be derived rigorously from the microstructure. Various particular cases of accurate models of acoustics and fluid filtration in rocks intensively studied by many authors: G. Nguetseng [9], J.L. Buchanan, R.P. Gilbert [10], M.J. Buckingham [11], R.P. Gilbert, A. Mikelic [12], T.H. Clopeau, J.L. Ferrin, R.P. Gilbert, A. Mikelic [13], J.L. Ferrin, A. Mikelic [14] and others. Detailed analysis can be found in [15], [16]. The most systematic investigations of accurate models of physical processes in poroelastic media were conducted by A.M. Meirmanov [16] - [18]. These models on the micro level are based on the known equations of continuum mechanics [19] and chemical laws.

The goal of this work is the numerical implementation of the one-dimensional problem. Using numerical simulation of the leaching process, we explore the changes of the free boundary over time and positions of the boundary at different values of the parameters in the system of differential equations.

2 Equations

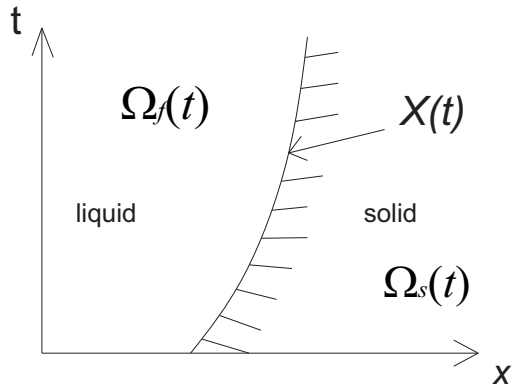

Figure 1 - One dimensional structure

For the case of one space variable differential equations for an incompressible fluid in the area $\Omega_f(t) = \{x : 0 < x < X(t)\}$ (see fig. 1) for $t > 0$ have the form

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

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

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

Boundary and initial conditions

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

$$\frac{dX}{dt} = \beta\,\gamma\,c, \;\; x = X(t), \;\; t > 0, \tag{5}$$

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

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

$$X(0) = X_0, \;\; c(x,0) = c_0(x), \;\; 0 < x < X_0. \tag{8}$$

Equations are written in dimensionless form. Here p is the pressure, v is the speed, c is the concentration of the active acid, $\alpha_c = \frac{DT}{L^2}$, D is the diffusion coefficient, T is the characteristic time, L is the characteristic size of the area, X is the free boundary, β, γ are given constants, ρ_s, ρ_f are dimensionless densities of the solid skeleton and liquid, respectively.

3 Numerical solution of the problem

For the numerical solution of the problem it is applied numerical simulation by finite difference method. Finite difference equations were derived using a simple explicit scheme. To solve the equation (6) at each time step Newton's method is used.

Finite-difference analog of the equation (3) is written as:

$$c_i^{n+1} = \frac{\alpha_c \triangle t}{h^2}(c_{i+1}^n - 2c_i^n + c_{i-1}^n) - v_l^n \frac{\triangle t}{h}(c_{i+1}^n - c_i^n) + c_i^n. \tag{9}$$

Finite-difference analog of the equation (6) is written as:

$$\frac{\rho_s}{\rho_f}\beta\gamma c_l^2 + (\beta + \frac{\alpha_c}{h})c_l - \frac{\alpha_c}{h}c_{l-1} = 0. \tag{10}$$

Applying the Newton's method, we rewrite equation (10):

$$c_l^{k+1} = c_l^k - \frac{\frac{\rho_s}{\rho_f}\beta\gamma(c_l^k)^2 + (\beta + \frac{\alpha_c}{h})c_l^k - \frac{\alpha_c}{h}c_{l-1}}{2\frac{\rho_s}{\rho_f}\beta\gamma c_l^k + \beta + \frac{\alpha_c}{h}}. \tag{11}$$

Here h is the spatial step size, the lower index i is the order of the nodes, the upper index n denotes a variable evaluated at the current time t and $n+1$ is a variable at the end of the time step (time $t + \triangle t$), k is the index of iteration and the lower index l denotes values at the free boundary.

By virtue of equations (2), (7) the speed of the liquid depends only on time. It is the same everywhere and equals to the speed at the free boundary. Therefore, the speed of the liquid at the free boundary is used in the equation (9).

For the exact description of the dynamics of the interface between the liquid and the solid skeleton, it is used interpolation method, which allows you to track the movement of the free boundary with sufficient accuracy. The method is implemented as follows. We know the initial position of the free boundary. We find regular grid nodes closest to the point of the free boundary and the values of the acid concentration in these nodes. Then, it is calculated the weighted value of the acid concentration at the free boundary by the found coordinates of points and values of the acid concentration. To distinguish the weighted value of the acid

concentration at the free boundary obtained by interpolation, let's denote it by c^X, ie with index X:

$$c^X = c_l^{k+1} + \frac{c_{l+1}^{k+1} - c_l^{k+1}}{h}(X^n - lh), \tag{12}$$

There is no acid concentration at the solid skeleton, so $c_{l+1}^{k+1} = 0$. Hence:

$$c^X = c_l^{k+1}(1 - \frac{X^n}{h} + l). \tag{13}$$

Interpolation can be done in different ways, in this case, linear interpolation is used. After determining the value of the acid concentration at the free boundary by the formula (13), the boundary can be moved. We find the new location of the free boundary using a simple explicit scheme:

$$X^{n+1} = \beta\gamma\triangle t c^X + X^n. \tag{14}$$

For $\gamma = 1$, $D = 2822\ \frac{\mu^2}{s}$, $L = 56$, $T = 0.00005\ s.$, and different values of β and c^+ we found the concentration c of active impurity on the free boundary and positions of the free boundary (fig. 1-4).

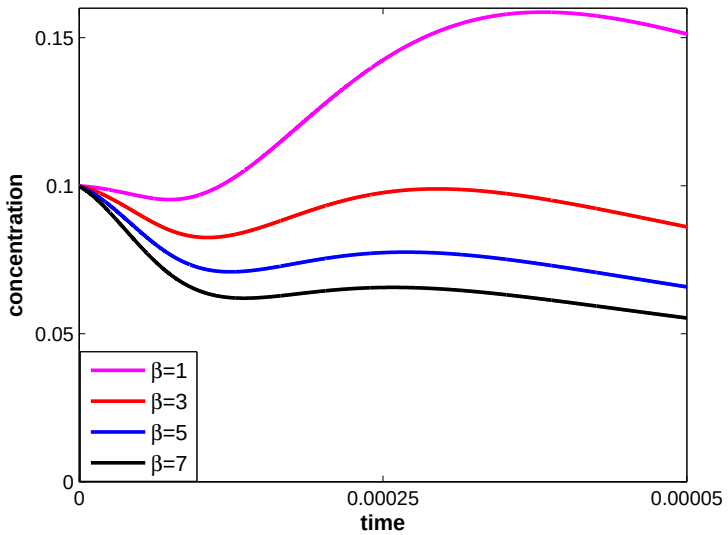

Figure 2 - Change of the active impurity concentration on the free boundary over time at various β

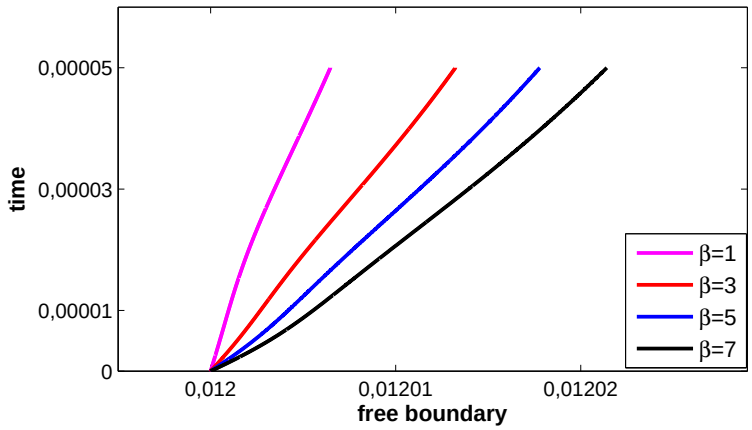

Figure 3 - Positions of the free boundary at various β

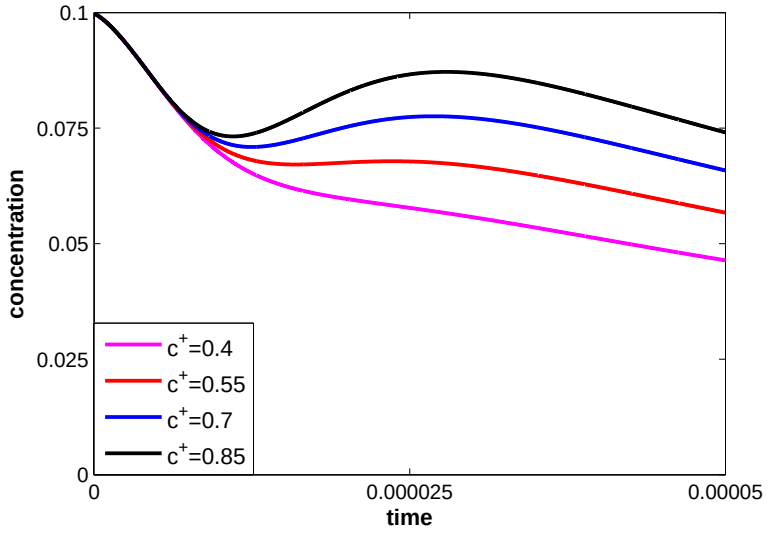

Figure 4 - Change of the active impurity concentration on the free boundary over time at various c^+

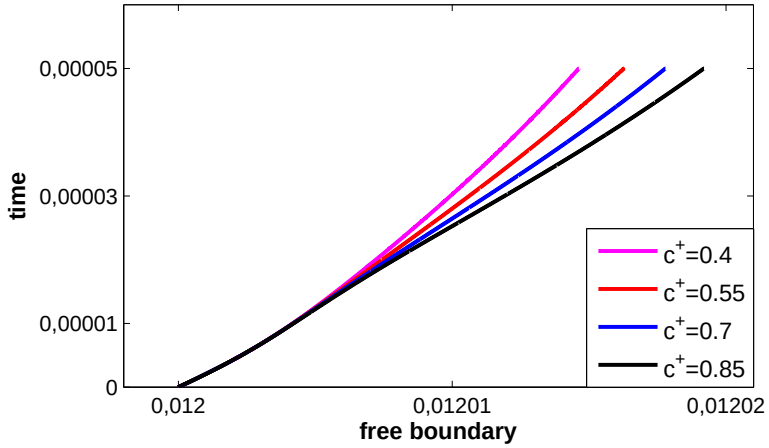

Figure 5 - Positions of the free boundary at various c^+

4 Conclusion

This article considers the numerical implementation of microscopic mathematical model describing the active impurity interaction with a solid skeleton. Numerical calculations of the one-dimensional problem implemented in Matlab mathematical environment. In numerical implementations you can see the distinctive features of the model. For example, smaller values of impurity concentration on the free boundary correspond to the greater values of the constant β (fig. 2). But the free boundary for a greater value β faster than the boundary for smaller β (fig. 3). It's quite a strange phenomenon for chemists. On the other hand, greater values of impurity concentration on the free boundary always correspond to greater values of concentration at the input c^+ (fig. 4), and the free boundary for greater value c^+ moves faster than the boundary for smaller c^+ (fig. 5).

From a practical point of view, the mathematical model is useful in possibility of studying the main features of the flow of physical and chemical processes on the free boundary between the liquid and solid skeleton.

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