S©MR ISSN 1813-3304

СИБИРСКИЕ ЭЛЕКТРОННЫЕ
МАТЕМАТИЧЕСКИЕ ИЗВЕСТИЯ

Siberian Electronic Mathematical Reports
http://semr.math.nsc.ru

*Том 13, стр. 726–733 (2016)* УДК 517.958:531.72
DOI 10.17377/semi.2016.13.057 MSC 76D27

# NUMERICAL MODELLING OF MICROSCOPIC DYNAMICS OF IN-SITU LEACHING

A.S. ZHUMALI, G.V. RESHETOVA

Abstract. Dissolution of the solid ground by an acid is one of subprocesses of in-situ leaching. The objective of this paper is the numerical simulation of these processes at the porous level. The case of two spatial variables is considered. We admit the fluid dynamics to be described by stationary Stokes equations, while acid concentration is described by the convection-diffusion equation. The problem is completed with boundary and initial conditions.

For the numerical simulation of the problem, the method of finite differences on staggered grids is used. At each time step, the fluid velocity components are computed iteratively by the successive over-relaxation method. The fluid pressure, the concentration of acid and the position of the free boundary are determined using an explicit scheme. To define the boundary condition for the acid concentration at the free boundary, a system of nonlinear equations is solved by the iterative Newton method.

Results of the numerical experiments are presented and discussed. In particular, the results obtained can help in analyzing the motion of the free solid/liquid interface and the mechanisms of physical and chemical processes there.

**Keywords:** leaching, free boundary, microscopic model, numerical solution.

## 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 carried out by injecting an acid to porous soil, wherein the acid reacts with the solid soil material. As a

Zhumali, A.S., Reshetova, G.V., Numerical modelling of microscopic dynamics of in-situ leaching.



The work was supported by Kazakh Fond of Fundamental Research (grant 1771/GF4).
*Received August, 5, 2016, published September, 16, 2016.*

result, the product of chemical interaction enters the liquid and the soil portion is dissolved.

This physical process is considered in a bounded volume, which consists of:

- the area simulating the pore space,
- the area simulating the solid skeleton,
- the boundary $X(y,t)$ between the pore space and the solid skeleton (Fig. 1).

The boundary $X(y,t)$ is unknown, since a part of soil is dissolved in the process of in-situ leaching, and the soil is deformed over time. Such problems are called free boundary problems.

Many authors investigated various special cases of exact models of fluid filtration in rocks. A detailed analysis can be found in [1]. The exact models of physical processes in porous media are systematically investigated in [2]. These models at the microscopic level are based on the known equations of continuum mechanics [3] and chemical laws [4].

The objective of this paper is the numerical implementation of algorithms for the description of in-situ leaching in the two-dimensional case. With the help of the numerical simulation the positions of the soil leaching boundaries at different values of parameters in the system of differential equations, and acid concentration at different time instants are investigated.

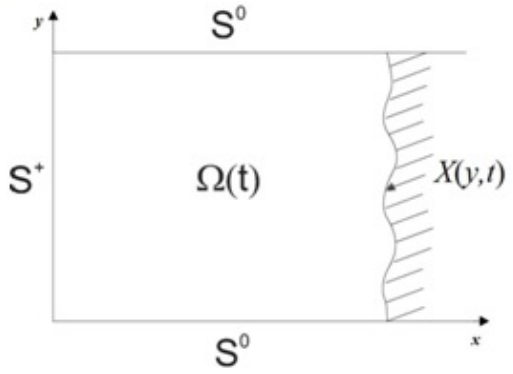


FIGURE 1. *The considered area*

## 2. Statement of the problem

The differential equations for the components of the velocity of the fluid, its pressure and acid concentration in the two-dimensional formulation have the following form:

- Two motion equations

$$\alpha_\mu \Delta \vec{v} - \nabla p = 0, \tag{1}$$

$$\varepsilon \frac{\partial p}{\partial t} + \nabla \cdot \vec{v} = 0, \tag{2}$$

- Transport equation for acid concentration

$$\frac{\partial c}{\partial t} + \vec{v} \cdot \nabla c = \alpha_c \Delta c, \tag{3}$$

- The boundary conditions at the free boundary $X(y,t)$ are:

$$(V_n + \beta - v_n)\, c + \alpha_c \nabla c \cdot \vec{n} = 0, \tag{4}$$

$$v_n = -V_n \frac{(\rho_s - \rho_f)}{\rho_f}\,, \tag{5}$$

where $V_n$ is the velocity of the free boundary in the direction of the outer normal $\vec{n}$, $v_n$ is the normal velocity of the fluid. The vector of the unit normal is as follows:

$$\vec{n} = \frac{1}{\sqrt{1 + \left(\frac{\partial X}{\partial y}\right)^2}} \left(1, -\frac{\partial X}{\partial y}\right).$$

- Velocity of a fluid coincides with the normal to an interface

$$\vec{v} - v_n\, \vec{n} = 0, \tag{6}$$

- The normal velocity of an interface is proportional to the acid concentration with some constants describing chemical kinetics

$$V_n = \beta \gamma\, c, \tag{7}$$

At the boundary $S^+$, which simulates the injection well, the normal stress in the fluid is proportional to the known pressure

$$(\alpha_\mu \mathrm{D}(\vec{v}) - p\mathrm{I}) \cdot \vec{n} = -p^+ \vec{n}, \tag{8}$$

$$c = c^+, \tag{9}$$

here I is the identity matrix and $\mathrm{D}(\vec{v}) = \frac{1}{2}(\nabla \vec{v} + \nabla \vec{v}^*)$.

At the liquid impermeable boundary $S^0$

$$\vec{v} = 0,\ \textit{and}\ \ \nabla c \cdot \vec{n} = 0. \tag{10}$$

The initial conditions:

$$X(y,0) = X_0, \quad c(x,y,0) = c_0(x,y), \quad (x,y) \in \Omega_0. \tag{11}$$

The equations are written down in the dimensionless form. Here $\alpha_\mu = \frac{\mu}{TLg\rho_0}$, $\varepsilon = \frac{gL}{c_s^2}$, $\alpha_c = \frac{DT}{L^2}$, $\mu$ is the viscosity coefficient, $g$ is the acceleration of gravity, $\rho_0$ is the water density, $c_s$ is the speed of sound in the fluid, $D$ is the diffusion coefficient, $T$ is the characteristic time, $L$ is the characteristic size of the area, $\beta$, $\gamma$ are the given constants characterizing the chemical process of interaction of

the acid with the rock, $\rho_s$, $\rho_f$ are the dimensionless densities of solid skeleton and fluid, respectively.

## 3. A numerical method

The numerical modeling is carried out by the finite difference method. The finite difference approximation of differential equations is constructed by the balance method on the rectangular staggered grids. To solve equation (**??**) at each time step the successive over-relaxation method (SOR) is used, and to solve equation (**??**) the Newton method is used.

After the application of the SOR method, the finite difference approximation of equation (**??**) componentwise takes the form:

$$v^{\alpha+1}_{x_{i+\frac{1}{2},j}} = (1-\omega)v^{\alpha}_{x_{i+\frac{1}{2},j}} + \frac{\omega}{2(\Delta x^2+\Delta y^2)}\times$$

(12)
$$\left[\left(v^{\alpha}_{x_{i+\frac{3}{2},j}} + v^{\alpha+1}_{x_{i-\frac{1}{2},j}}\right)\Delta y^2 + \left(v^{\alpha}_{x_{i+\frac{1}{2},j+1}} + v^{\alpha+1}_{x_{i+\frac{1}{2},j-1}}\right)\Delta x^2 - \Delta x\Delta y^2\frac{p_{i+1,j}-p_{i,j}}{\alpha_\mu}\right].$$

$$v^{\alpha+1}_{y_{i,j+\frac{1}{2}}} = (1-\omega)v^{\alpha}_{y_{i,j+\frac{1}{2}}} + \frac{\omega}{2(\Delta x^2+\Delta y^2)}\times$$

(13)
$$\left[\left(v^{\alpha}_{y_{i+1,j+\frac{1}{2}}} + v^{\alpha+1}_{y_{i-1,j+\frac{1}{2}}}\right)\Delta y^2 + \left(v^{\alpha}_{y_{i,j+\frac{3}{2}}} + v^{\alpha+1}_{y_{i,j-\frac{1}{2}}}\right)\Delta x^2 - \Delta x^2\Delta y\frac{p_{i,j+1}-p_{i,j}}{\alpha_\mu}\right].$$

where $\omega$ is the relaxation parameter $(1<\omega<2)$.

The finite difference analogue to equation (**??**):

(14)
$$p^{n+1}_{i,j} = p^{n}_{i,j} - \frac{\Delta t}{\varepsilon}\left[\left(v^{n+1}_{x_{i+\frac{3}{2},j}} - v^{n+1}_{x_{i-\frac{1}{2},j}}\right)\Big/(2\Delta x) + \left(v^{n+1}_{y_{i,j+\frac{3}{2}}} - v^{n+1}_{y_{i,j-\frac{1}{2}}}\right)\Big/(2\Delta y)\right].$$

The finite difference analogue to equation (**??**):

$$c^{n+1}_{i,j} = c^{n}_{i,j} + \Delta t\alpha_c\left[\frac{c^{n}_{i+1,j}-2c^{n}_{i,j}+c^{n}_{i-1,j}}{\Delta x^2} + \frac{c^{n}_{i,j+1}-2c^{n}_{i,j}+c^{n}_{i,j-1}}{\Delta y^2}\right] -$$

(15)
$$\Delta t\left[v^{n+1}_{x_{i+\frac{1}{2},j}}\frac{c^{n}_{i+1,j}-c^{n}_{i,j}}{\Delta x} + v^{n+1}_{y_{i,j+\frac{1}{2}}}\frac{c^{n}_{i,j+1}-c^{n}_{i,j}}{\Delta y}\right]$$

The finite difference analogue to equation (**??**):

(16)
$$\frac{\rho_s}{\rho_f}\beta\gamma c^2_{N,0} + \beta c_{N,0} + \alpha_c\frac{c_{N,0}-c_{N-1,0}}{\Delta x\sqrt{1+\left[\left(X_1-X_0\right)/\Delta y\right]^2}} = 0, \quad at\ \ y=0,$$

(17)
$$\frac{\rho_s}{\rho_f}\beta\gamma c^2_{N,M} + \beta c_{N,M} + \alpha_c\frac{c_{N,M}-c_{N-1,M}}{\Delta x\sqrt{1+\left[\left(X_M-X_{M-1}\right)/\Delta y\right]^2}} = 0, \quad at\ \ y=y_M,$$

$$c_{N,j+1} = c_{N,j} + \beta\,\Delta y^2\frac{\sqrt{1+\left[\left(X_{j+1}-X_j\right)/\Delta y\right]^2}}{\alpha_c\left(X_{j+1}-X_j\right)}\left(\frac{\rho_s}{\rho_f}\gamma c^2_{N,j} + c_{N,j}\right) +$$

$$\frac{\Delta y^2}{\Delta x\left(X_{j+1}-X_j\right)}\left(c_{N,j}-c_{N-1,j}\right), \quad at \;\; y=\overline{y_1,y_{M-1}}. \tag{18}$$

Equations (**??**) and (**??**) are solved by the Newton method:

$$c_{N,0}^{k+1}=c_{N,0}^{k}-\left\{\frac{\rho_s}{\rho_f}\beta\gamma c_{N,0}^2+\beta c_{N,0}+\alpha_c\frac{c_{N,0}-c_{N-1,0}}{\Delta x\sqrt{1+\left[\left(X_1-X_0\right)/\Delta y\right]^2}}\right\}\Bigg/$$

$$\left\{2\beta\gamma\frac{\rho_s}{\rho_f}c_{N,0}+\beta+\frac{\alpha_c}{\Delta x\sqrt{1+\left[\left(X_1-X_0\right)/\Delta y\right]^2}}\right\}, \tag{19}$$

$$c_{N,M}^{k+1}=c_{N,M}^{k}-\left\{\frac{\rho_s}{\rho_f}\beta\gamma c_{N,M}^2+\beta c_{N,M}+\alpha_c\frac{c_{N,M}-c_{N-1,M}}{\Delta x\sqrt{1+\left[\left(X_M-X_{M-1}\right)/\Delta y\right]^2}}\right\}\Bigg/$$

$$\left\{2\beta\gamma\frac{\rho_s}{\rho_f}c_{N,M}+\beta+\frac{\alpha_c}{\Delta x\sqrt{1+\left[\left(X_M-X_{M-1}\right)/\Delta y\right]^2}}\right\}. \tag{20}$$

Using a simple explicit scheme we find the new location of the free leaching boundary:

$$X_j^{n+1}=\beta\gamma\Delta t c_{N,j}^{n+1}\sqrt{1+\left[\left(X_{j+1}-X_j\right)/\Delta y\right]^2}+X_j^n \tag{21}$$

## 4. The results of numerical experiments

The numerical solution for microscopic mathematical model describing the interaction of active impurity with a solid skeleton was obtained.

Calculations of modeling the position of the free boundary and impurity concentration for different time for the following parameters of the model

$$\gamma=1, D=2822\,\frac{\mu m^2}{s}, L=56\mu m, H=42\mu m, T=0.01\,s.$$

and for different values of $\beta$, $c^+$ are presented in Figs. 2-5.

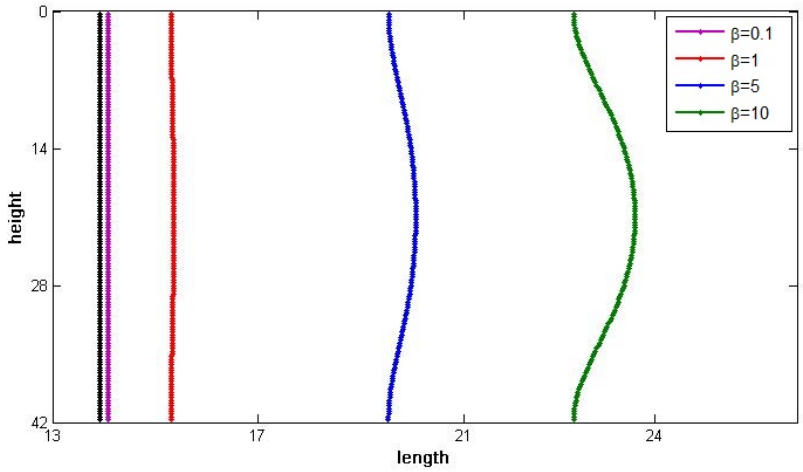


FIGURE 2. *The position of the free boundary at different* $\beta$

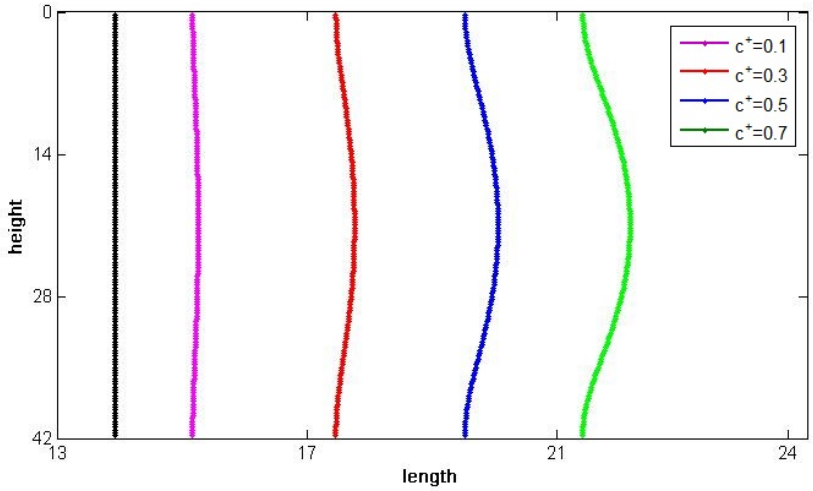


FIGURE 3. *The position of the free boundary at different* $c^+$

In Figure 2, the black line shows the initial position of the free boundary, and the other lines represent the positions of the free boundary at the time $T = 0.01\,s.$ for different values of the chemical reaction coefficient $\beta$. In Figure 3, the black line shows the initial position of the free boundary and the other lines represent the positions of the free boundary at the time $T = 0.01\,s.$ for different values of the acid concentration $c^+$ at the inputting boundary. Free boundary for a greater value of the constant $\beta$ moves faster than the boundary for a smaller $\beta$ (Fig. 2). When supplying a greater concentration $c^+$ at the inputting boundary, the soil is dissolved faster than at lower values of $c^+$ (Fig. 3). Figure 4 shows the acid diffusion for different moments of time at a constant acid concentration corresponding to $c^+$

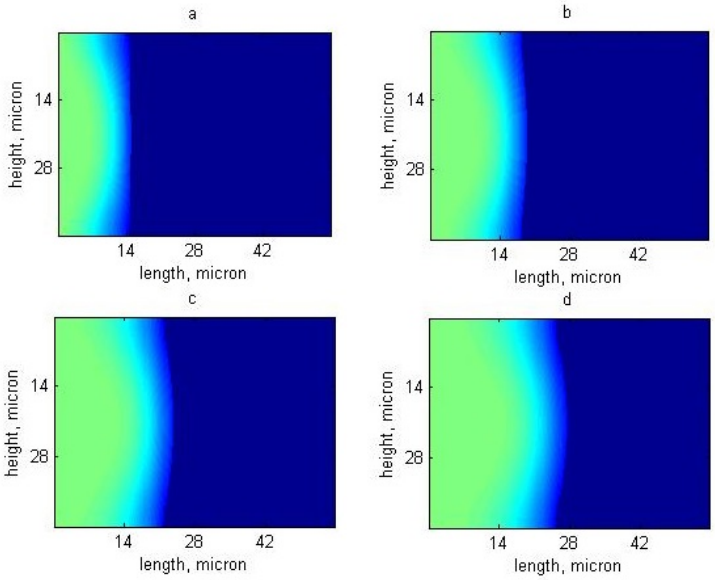


FIGURE 4. *The acid concentration at different time moments: a - 0.0028 s., b - 0.0036 s., c - 0.0044 s., d - 0.0052 s.*

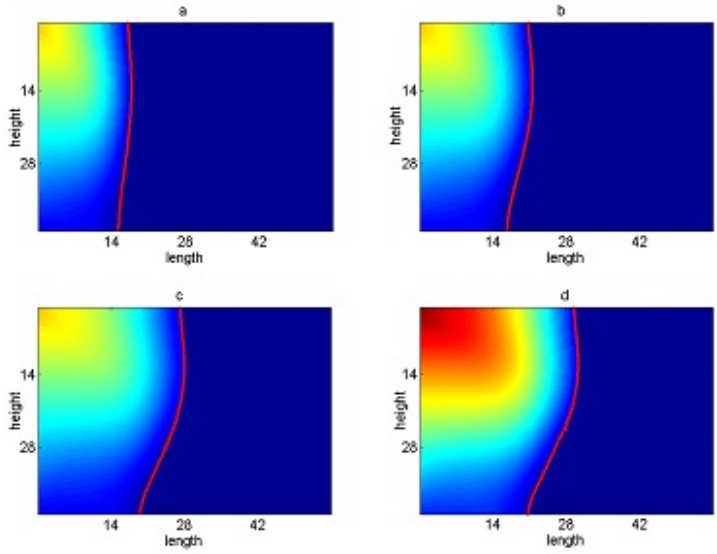


FIGURE 5. *The acid concentration at different time moments when* $c^+ = 0.7 - y_j/dy$*: a - 0.0028 s., b - 0.0036 s., c - 0.0052s., d - 0.0064s.*

(with $\beta = 100$). Figure 5 shows the acid diffusion for different moments of time when $c^+$ is dependent on the vertical coordinate $y$ (with $\beta = 100$).

## 5. Conclusion

This paper deals with a numerical solution of the microscopic mathematical model describing the active impurity interaction with a solid skeleton. The finite difference equations based on the balance method are derived and the algorithm of the numerical solution based on a combination of the SOR, the Newton method and explicit difference equations are proposed. The results of the calculations and the numerical performance analysis are presented.

## References

[1] R. Burridge, G.B. Keller, *Poroelasticity equations derived from microstructure* , Journal of Acoustic Society of America, (1981), 1140–1146. Zbl 0519.73038
[2] A. Meirmanov, *Mathematical models for poroelastic flows*, AtlantisPress, Paris, 2013.
[3] L.V. Ovsyannikov, *Introduction to continuum mechanics*, Novosibirsk State University, Novosibirsk, 1977.
[4] N.L. Glinka, *General chemistry*, Integral-press, Moscow, 2005.

Ainur Serikbaykyzy Zhumali
Kazakh-British Technical University,
Tole bi st., 59,
050000, Almaty, Kazakhstan
*E-mail address*: ainura.z89@gmail.com

Galina Vitalevna Reshetova
Institute of Computational Mathematics and Mathematical Geophysics SB RAS,
prospect Akademika Lavrentjeva, 6,
630090, Novosibirsk, Russia
*E-mail address*: kgv@nmsf.sscc.ru