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STUDY OF IN-SITU LEACHING OF METALS BY NUMERICAL SIMULATION

Abstract. The article is devoted to numerical modeling of uranium in-situ leaching process, which enables to assess the dynamics of the technological process. Efficient simulation of in-situleaching is an urgent task, demanded by many enterprises of the mining industry worldwide. Mathematical modeling, given in the article, describes the dynamics of in-situ leaching. It should be borne in mind that in-situ leaching has characteristics, in connection with which its use becomes specific, it requires some knowledge and tools for analysis and management process. Designed to be a conceptual model allows to take into account all the information about the geological environment, the geometrical properties of hydraulic parameters of solid state properties, including homogeneous and isotropic, fluid properties, boundary conditions.

Keywords: in-situ leaching, conceptual model, numerical modeling, mathematical modeling, Darcy law, visualization.

Introduction. More and more attention is paid to modeling of the in-situ leaching process with the aim of solving problems to raise the efficiency of the process.

The peculiarity of the process of in-situ leaching (ISL) is determined by liquid filtration processes in the soil. The permeability of the ore and host rocks is one of the most important conditions for the movement of leaching solutions, so when modeling ISL processes, the study of filtration properties is one of the main tasks.

Quantitatively, the permeability of the ore and host rock is expressed by coefficient of permeability or the coefficient of permeability to water, which is numerically equal to the rate of water filtration through the rock when the pressure gradient equal to unity, and is measured in m/day (or cm/s). Of great importance is the filtration heterogeneity of ores and ore-bearing rocks, which determines the convective dispersion and distribution of solutions, and also controls the mass transfer in the productive strata.

Development of a numerical model can be described as a representation of the conceptual model of natural systems with the use of numerical algorithms of in-situ leaching and groundwater interaction.

Numerical models are used to simulate the system perturbation to assess more complex real systems.

Using the basic laws of physics and chemistry that govern the groundwater flow and solute necessary to develop a mathematically represented the conceptual model. Conceptual model includes all the information about the geological conditions, geometric properties, hydraulic parameters, solid state properties, including the homogeneity and isotropy, liquid properties, boundary conditions as sources and sinks of liquids, solutes, as well as their spatial dependent on time distributions within the study area and its boundaries. The aim of the numerical model is a solution of the differential equation in stationary conditions for the unperturbed system and allows to simulate the behavior of the process over time.

Identification of the specific objectives of the model.

• Development of a conceptual model of in-situ leaching, which includes all available information on the hydrodynamic and geochemical data on the physical and chemical properties of the system that are relevant for the explicit description of the system. These are the properties that describe the movement of groundwater and solutions and mass transfer.

• Mathematical modeling, where all the concepts of conceptual model are expressed in mathematical equations. Assumptions about the boundary conditions and other properties of the conceptual model are also included.

• Development of numerical model (1) Discretization of the field of numerical grid or grid from the field, in order to simulate, or use other discretization methods, such as meshless methods;

(2) Discretization of the mathematical equations of the mathematical model (if you write your own computer simulation program), or choose a computer program that can solve the mathematical equations of the mathematical model. Computer software should be checked against the known analytical solutions or previously solved problems, to determine whether the computer code is correctly and functioning properly. The contribution of the program are assigned values of hydraulic parameters, fluid and material properties, etc., each element or element; (3) Assignment of boundary conditions to the grid or the mesh (external and internal).

• Calibration of the numerical model, wherein the numerical values of physical parameters of simulation in the computational model are optimized in such a way that a good match between the simulated and measured data of the field is achieved, and the results are plausible. Model calibration is performed using field data collected in the past and compared with the numerical results.

• Checking numerical model is used to determine the extent to which the model is an accurate representation of the real world in terms of the intended use of the model. This is accomplished using the field data which have not yet been used to calibrate the model.

• After calibration and validation, sensitivity analysis is to identify the most important parameters that affect the behavior of the system. If the uncertainty of the model is low (comparing numerical results with experimental data), numerical model can be considered suitable to carry out the numerical simulation in accordance with the specific tasks for which it was designed (for example, to make predictions).

This article describes the steps to create the model, the steps of creating a model are presented, see Figure 1.

1. Defining goals of numerical model. Numerical models are used to perform simulations for the recovery processes that occurred in the past and predict the processes of subsurface complex systems, such as in-situ leaching, or fluid movement in porous media in which multiple connected processes with interactive parameters and functions of parameters of movement of in-situ rocks and water, and transport of solutes and solutions.

2. Conceptual model. Before choosing commercial software or creating a custom built-in code for development of a digital model, conceptual model of the subject area to be created. The conceptual model is our idealization of the hydrogeological system described by a mathematical and numerical models. It is a virtual representation of the geological system, relying on maps, sections and existing databases, such as the physical and chemical properties, provides a clear description of the most important properties that control the flow of the solution and dissolved substances. The conceptual model includes assumptions about (1) regulating processes related to groundwater, solute, (2) transport on the borders of the region, (3) dimension, (4) hydro-stratigraphy, (5) the flow direction (6) material properties, and (7) pattern heterogeneity. In other words, the conceptual model is a simplified representation of systematic and high-level area containing a set of assumptions. This model represents the best understanding of the processes that occur naturally in in-situ leaching.

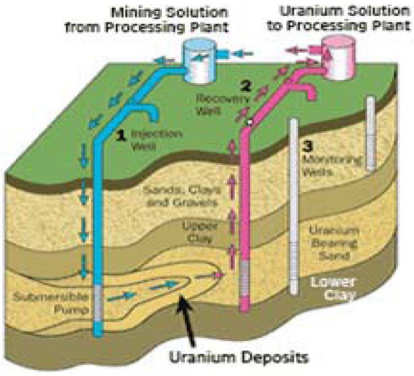
3. The method of in-situ leaching develops exogenous uranium deposits that are on highly permeable underground water levels. The extraction of uranium from the ore body occurs through a system of technological wells, Figure 2. After the injection wells (1) into a productive horizon the substances solution flows capable of dissolving the uranium-containing minerals. Resulting in underground water level productive solution is extracted through an exhaust hole (2). Formed after the processing of productive solutions, stock solutions are consolidated by leaching reagents and again fed into the injection wells as working solutions. The main objectives of management geotechnological enterprise is to increase the profitability of the field development, an increase in the proportion of uranium extracted from the productive horizon, and the reduction of groundwater pollution. To solve this problem it is necessary to be able to evaluate geochemical and hydrogeological state of the productive horizon and groundwater.

Procedure of a numerical model elaboration

1. Defining specific objectives of the model

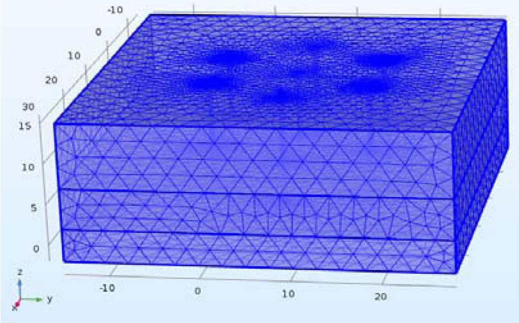
Data collection and compiilation

2. Conceptual model



3. Numerical model

Discretization of model area



Discretizing the mathematical equations

$$\frac{\partial h}{\partial x}(x_0, y_0) = \frac{h(x_0 - \Delta x, y_0) - h(x_0, y_0)}{\Delta x}$$

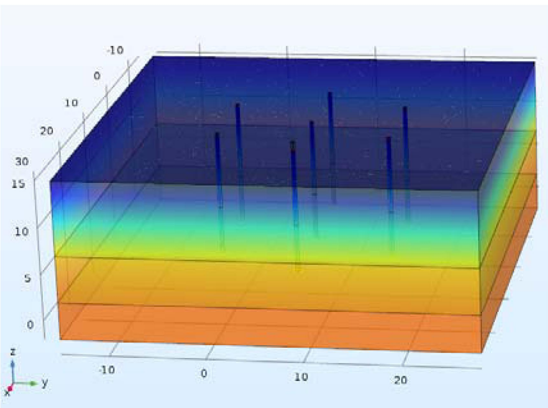
$$\frac{\partial^2 h}{\partial x^2}(x_0, y_0) = \frac{\frac{\partial h}{\partial x}(x_0 - \Delta x, y_0) - \frac{\partial h}{\partial x}(x_0, y_0)}{\Delta x}$$

4. Mathematical model

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = 0$$

$$K_x \frac{\partial^2 h}{\partial x^2} + K_y \frac{\partial^2 h}{\partial y^2} = S_s \frac{\partial y}{\partial x}$$

5. Results modeling



6. Process Visualization

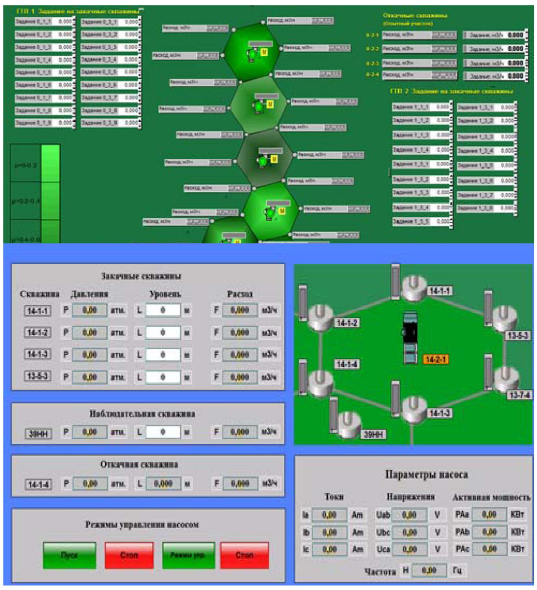


Figure 1 – Stages of creating a model

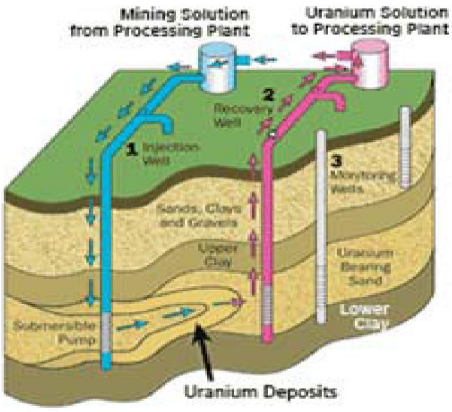


Figure 2 – Conceptual model

Around each mineralization zone observation wells group is drilled (3) to monitor the movement of solutions beyond the area of deposit. Wells are socketed for fluid to be flowed only in the ore zone and out of it, without touching the underground water levels.

4. Mathematical modeling. After the acquisition of information and field data on the water level system it is a creation of the conceptual model, which have been identified and expressed their basic equations, related transport processes in the subsurface. Then, the program selection for evaluation of the modeling process. Validation of each individual program, in accordance with the available field data and modeling tasks is needed before the selection of the final program.

The main objectives of the modeling are:

- for evaluating in-situ fluids flow parameters by comparing numerical results with measurement data of experiment

- for predicting the flow tendencies.

The mathematical formulation of the problem. Mathematical model of single-phase flow in porous media is described by the continuity equation

$$\frac{\partial m\rho}{\partial t} + \mathrm{div}\rho u = f(x,t) \qquad (1)$$

and by Darcy law

$$u = -k\mu(\mathrm{grad}\, p + \rho \mathrm{g}), \qquad (2)$$

where p – pressure, u – filtration rate of the fluid in a porous medium, k – permeability of a porous medium, μ – fluid viscosity, g – gravity vector and f – the density of internal sources / sinks.

Substituting Darcy law (2) into the continuity equation (1), taking into account the poor compressibility of the fluid, the elastic deformability of the collector and neglecting the influence of gravitational forces due to low power of oilfields [7-9] (layer thickness by 2-3 orders lower than the characteristic dimensions of the reservoir in the horizontal plane), we have the following equation for the pressure:

$$\beta\frac{\partial p}{\partial t} - \mathrm{div}\left(\frac{k}{\mu}\,\mathrm{grad}\, p\right) = f(x,t), \qquad (3)$$

where β – coefficient of joint compressibility of fluid and collector.

In computational practice of filtration solution the right side f (x,t) can be defined as the sum of the sources/sinks capacity

$$\frac{\partial p}{\partial t} - \mathrm{div}\left(\frac{k}{\mu}\,\mathrm{grad}\, p\right) = \sum_{i=1}^{N_q} q_i(t)\,\psi_i(x), x \in \Omega, t \in (0,T], \qquad (4)$$

where q_i for two-dimensional case, when setting pointed source/sink - i-th discharge borehole, and in the case of horizontal wells - the fluid inflow per unit of surface of the i-th wellbore, $\psi_i(x)$ – non-negative weight function, N_q – quantity of wells, T > 0 and $\Omega \in R^{\alpha}$, α = 2, 3.

Equation (4) is supplemented by appropriate boundary and initial conditions

$$-\frac{k}{\mu}\frac{\partial p}{\partial n} = 0, x \in \Gamma, t \in (0, T], \quad (5)$$

$$p(x, 0) = p_0(x), x \in \Omega, \quad (6)$$

where Γ – boundary Ω, *n* – external normal to Γ.

Thus, it is required to find the function $p(x, t)$, $t \in (0, T], T > 0$, satisfying the parabolic equation, boundary and initial conditions (5), (6) at the given input $k, \mu, c, p_0, q_i(t), \psi_i(x), i = 1, 2, \ldots, N_q$. Initial boundary value problem (4)-(6) belongs to the class of direct problems.

5. Numerous setting of the conceptual model. After the conceptual model is built, all the information contained in it should be converted into a set of mathematical expressions, expressing the mass of dissolved substances and the energy balance and flow of equations (including the relevant boundary conditions). Then, a numerical model is constructed by discretization of these mathematical equations in space, using a volume management approach, and in time. The resulting matrix of discrete numerical equations and sets of the input data with the boundary and initial conditions are used for the numerical simulation of the responses to the real system. The values of the input variables can be modified to produce different simulation scenarios.

The data management approach uses the grid, ie the field of discrete cells that covers the domain model in one, two or three dimensions. To control the volume of each element individual averaging (or interpolation) of flow, transport and thermodynamic properties and variables is performed. Volume management approach includes the following commonly used sampling schemes: the usual method of finite differences, different methods of finite elements, e.g., the classical Galerkin methods of finite element, as well as boundary element and methods of meshless that have been developed in recent years and are used for UL simulation.

6. Modeling in the comsol multiphysics. To solve the PDE, COMSOL Multiphysics uses the finite element method (FEM). The software runs the finite element analysis, together with the grid taking into account the geometrical configuration of bodies, and error control using a variety of numerical solvers. Since many of the physical laws are expressed in the form of PDE, it is possible to simulate a wide range of scientific and engineering phenomena of many areas of physics such as chemical reaction, diffusion, hydrodynamics, filtration etc.

In addition to the above mentioned, the program allows with the help of coupling variables to connect the models in different geometries and to link models of different dimensions.

Comsol Multiphysics is used for the numerical simulation of flow distribution for analytical solutions, as well as the use of different modes for the simulation experiment. As a starting point there are the boundary and initial conditions.

Schematic representation of the profile of the hexagonal cell shape of leaching is shown in the figure.

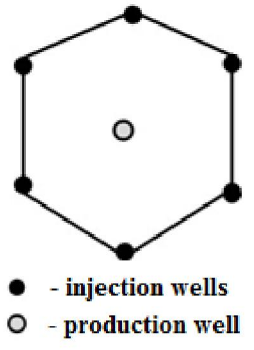


Figure 3 – Schematic representation of the hexagonal UL

Numerical modeling consists of several steps:

- Choice of physical law for the modeling process;
- Choice of methods for solving differential equations in partial derivatives;
- Carrying out the construction of geometry;
- Preparation of research results.

1. Selection of Physics. As a selected physical law it is an empirical Darcy law (2) in a porous medium of non-isothermal fluids to determine the hydraulic pressure.

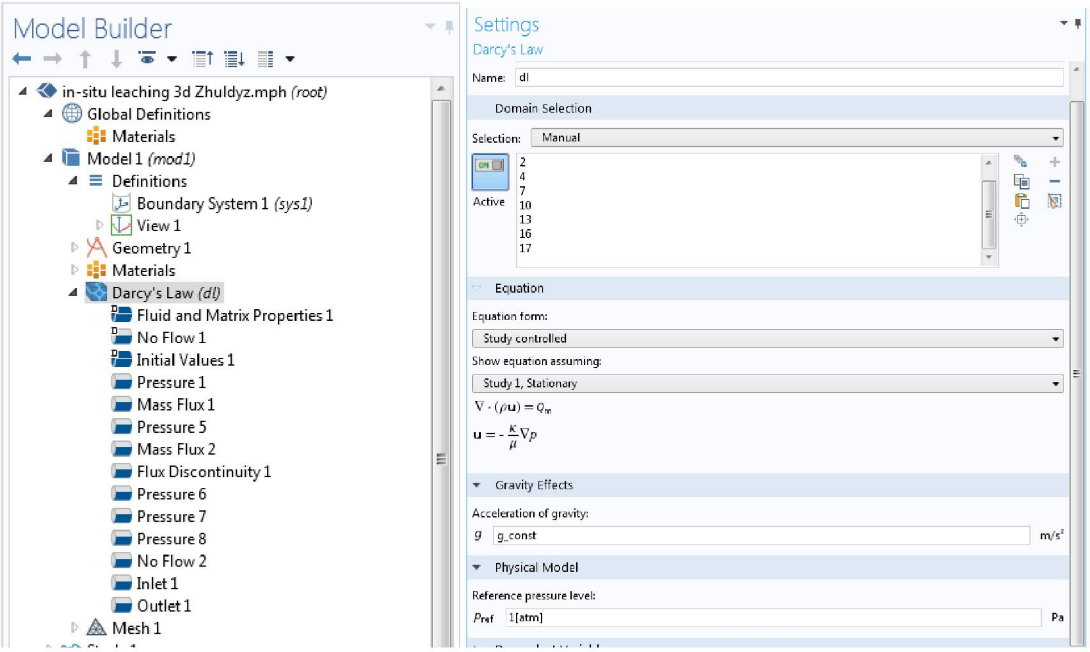
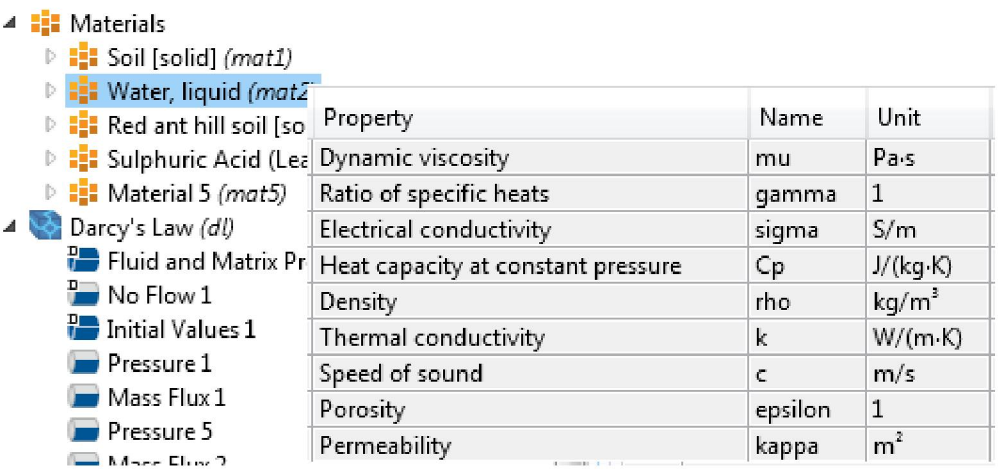


Figure 4 – Selecting the physical law for modeling

2. The PDE method. For the numerical solution of differential equations in partial derivatives it was chosen the Lagrange-Euler method of arbitrary calculating to calculate the change in the flow of underground fluids in space and in time with the given initials and boundary conditions.



Picture 5 – Set initial conditions

3. Construction of geometry. The presented 3D-model is conditionally divided into three layers: the bottom two layers are porous media with different degrees of permeability, the upper layer is an imitation of the liquid column of groundwater (figure 6).

4. Simulation results. The kinetics of the process is determined by mass transfer of the solvent and the dissolved uranium, due in turn to their concentration gradient.

The most important parameter that determines the kinetics of uranium leaching from massive ores with artificial permeability is the rate of solvent penetration into the ore monolith. It depends on the number and size of pores and capillaries in the ore monolith and their degree of structural changes in the leaching process.

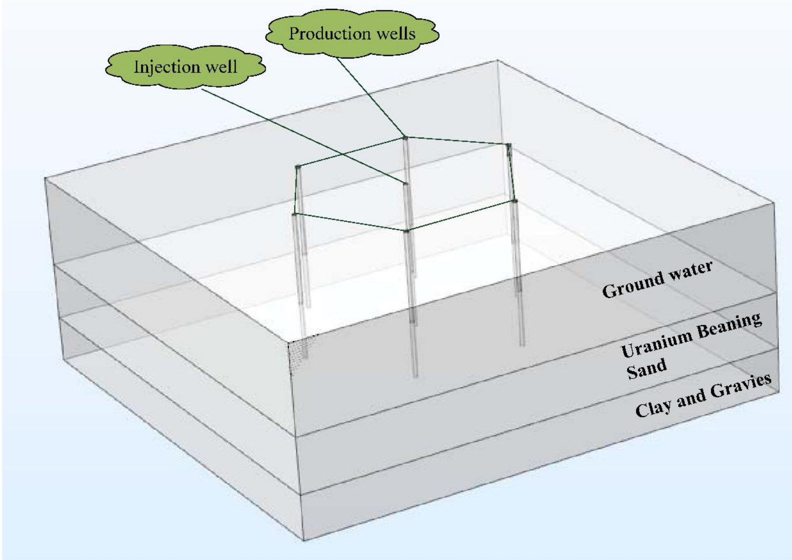


Figure 6 – Constructing 3D geometry

These changes are usually caused by the ore material composition and the nature of its interaction with the solvent. The formation and deposition in the pores of secondary chemical compounds can alter the kinetics of uranium leaching. Particularly unfavorable ores are those containing carbonate minerals: in their solutions of sulfuric acid processing it is the formation of sparingly soluble gypsum, bridging the pores and capillaries.

By the nature of the solvent penetrating into piece ores are divided into the following three types:

1. Ores in which solvent leaks more or less simultaneously and continuously on all sides;

2. Ores, in which solvent penetrates firstly through cracks and lamination planes, ie, on the main channels and then is fed into the smallest pores and capillaries;

3. Ores, which when solvent processing are destroyed.

Porosity of ore monoliths is typically many times less than the porosity of clay, but the size of pores and capillaries in the piece is higher than in clay formations.

As is seen from the simulation results in Comsol environment shown in Figures 7-10 of the leaching in stationary modes it is observed symmetrical patterns of filtering process with the formation of stagnant zones of the process.

To eliminate stagnant zones it is recommended to constantly change the leaching regime in wells.

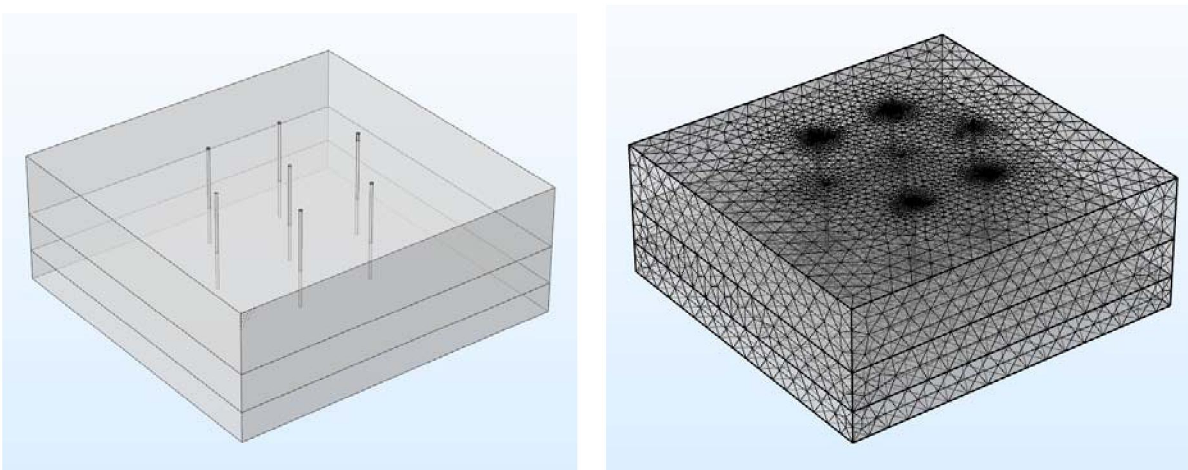


Figure 7 – Construction of the geometry of the simulated object and the partition into the grid

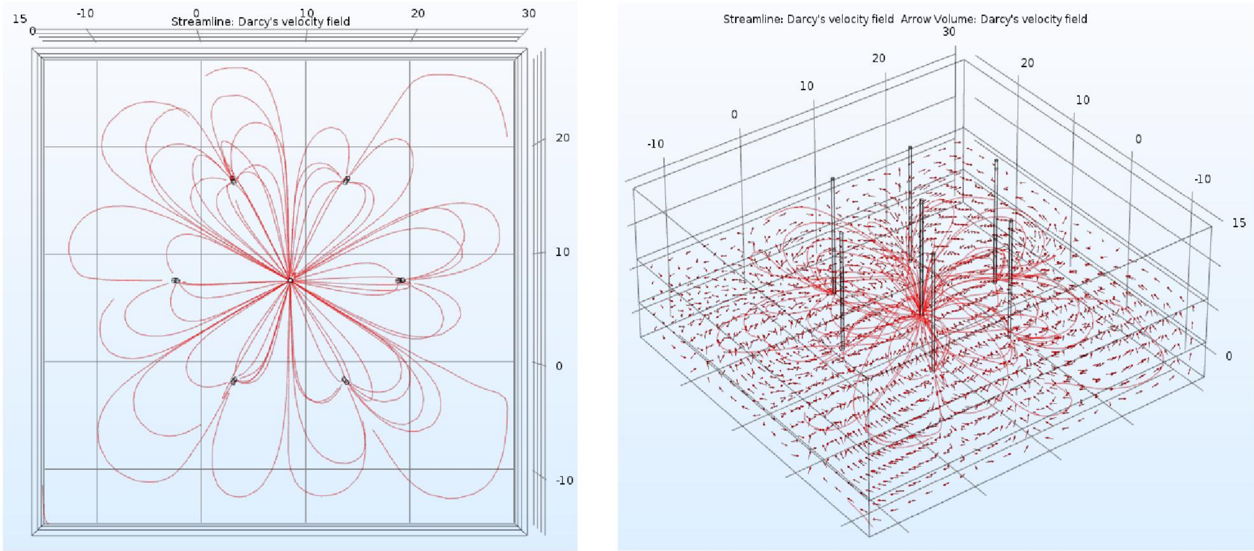


Figure 8 – Distribution of hydrodynamic pressure field between the pumping and injection wells

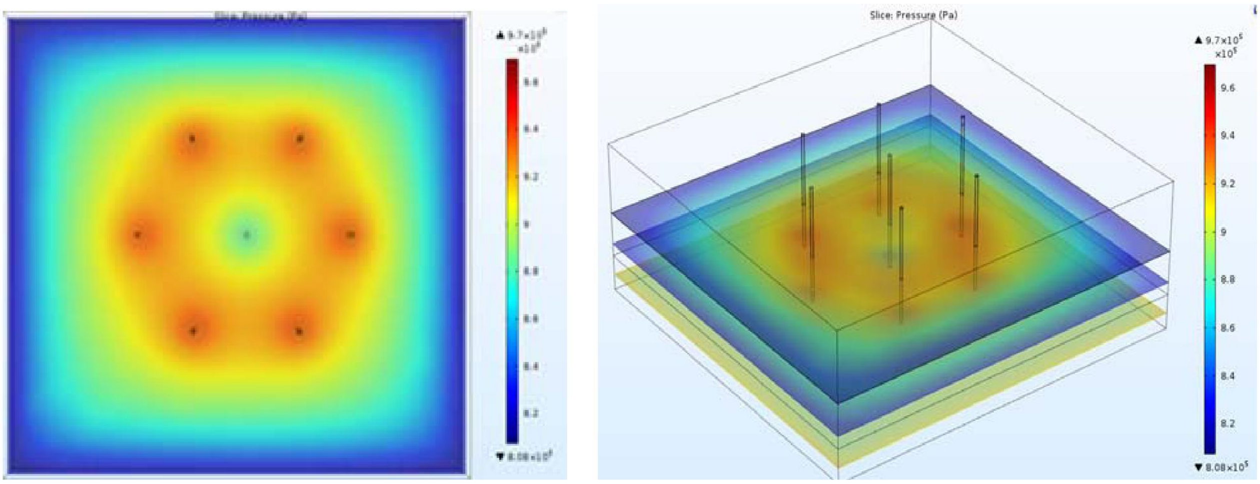


Figure 9 – Pressure distribution circuit

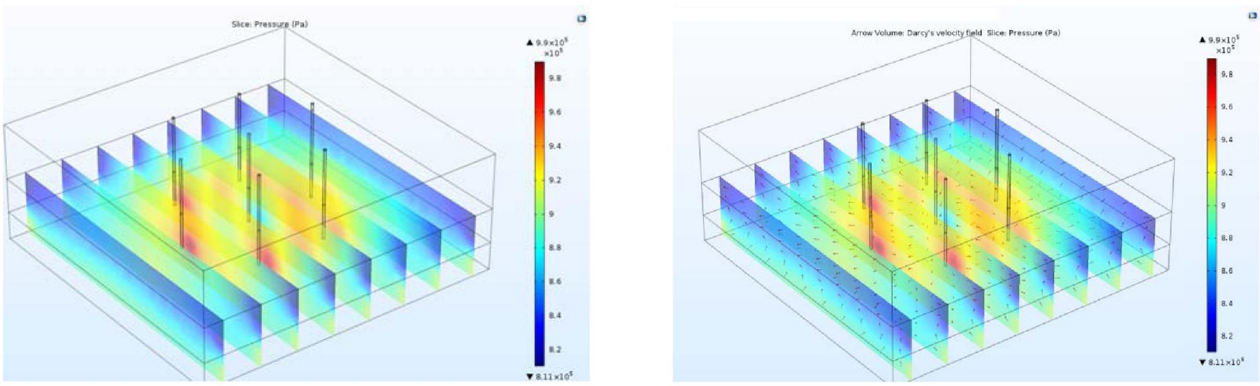


Figure 10 – Circuit the pressure distribution over the layers

7. The visualization process. The advantage of modern visual systems is that they not only display a static state of the object, but also allow to:

- observe the process in dynamics;
- archive process variables, and then print them in the form of reports;

- manage the process from the PC screen or operator panels via mouse and keyboard;
- print the forms of reports and assignments;
- change the process parameters via PC or OP;
- make changes in production;
- store in PC memory modes and recipes of production;
- issue posts by specified events.

Also it allows to quickly and analytically process the collected data.

Conclusion. As in the case of the percolation, in in-situ uranium leaching of ores with natural permeability transport of solvent to the surface and the dissolved reaction products from the interaction surface is determined by the rate of infiltration of solutions. The reaction between the liquid solvent and the solid particle develops from the surface to the center, and till complete leaching the unreacted core remains at the center and on the surface - a solid.

Ore material, having a porous structure, complicates the process of diffusion, putting a resistance. The smaller diffusion resistance, the higher the leach rate and degree of uranium leaching process in a predetermined duration.

Simulation analysis shows that the process of leaching the overwhelming part of uranium minerals from ores with natural permeability is determined by the laws of diffusion kinetics as the controlling factor in the overall speed of the mass transfer and the laws of hydrodynamics, which allows a quantitative assessment of the leaching rate.

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САНДЫҚ МОДЕЛЬДЕУ КӨМЕГІМЕН МЕТАЛДАРДЫ ЖЕР АСТЫ СІЛТІСІЗДЕНДІРУ ПРОЦЕСІН ЗЕРТТЕУ

Аннотация. Мақала технологиялық пропроцестің динамикасын бағалауға мүмкіндік беретін уранды жер асты сілтісіздендіру процестерін жер асты сандық модельдеуге арналған. Жер асты сілтісіздендіру процесін тиімді модельдеу бүкіл әлемдегі тау-кен қазу кәсіпорындарының көбісінде сұранысқа ие өзекті тапсырма болып табылады. Мақалада келтірілген математикалық модельдеу жер асты сілтісіздендіру динамикасын сипаттайды. Соның өзінде де, жер асты сілтісіздендіруінің өзіндік ерекшеліктері бар екендігін ескерген жөн, соған байланысты оны қолдану спецификалық болып келеді, процесті талдау және басқару үшін нақты білімдер мен құрал-жабдықтарды талап етеді. Мақалада жасалынған концептуалды модель геологиялық жағдай, геометриялық қасиеттер, гидравликалық параметрлер, қатты фазалық қасиеттер, соның ішінде біртектілік пен изотроптылық, сұйықтың қасиеттері, шекаралық жағдайлар туралы барлық ақпаратты ескеруге мүмкіндік береді.

Түйін сөздер: жер асты сілтісіздендіру, концептуалды модель, сандық модельдеу, математикалық модельдеу, Дарси заңы, визуализация.

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ИССЛЕДОВАНИЕ ПРОЦЕССА ПОДЗЕМНОГО ВЫЩЕЛАЧИВАНИЯ МЕТАЛЛОВ С ПОМОЩЬЮ ЧИСЛЕННОГО МОДЕЛИРОВАНИЯ

Аннотация. Статья посвящена численному моделированию процессов подземного выщелачивания урана, которое позволяет оценивать динамику технологического процесса. Эффективное моделирование процесса подземного выщелачивания является актуальной задачей, востребованной многими предприятиями горнодобывающей отрасли во всем мире. Математическое моделирование, приведенное в статье, описывает динамику подземного выщелачивания. При этом необходимо учитывать, что подземное выщелачивание имеет характерные особенности, в связи, с чем его применение становится специфичным, требует определенных знаний и инструментов для анализа и управления процессом. Разработанная в статье концептуальная модель позволяет, учитывает всю информацию о геологической обстановке, геометрических свойств, гидравлических параметров, твердофазных свойств, в том числе однородности и изотропности, свойств жидкости, граничного условия.

Ключевые слова: подземное выщелачивания, концептуальная модель, численное моделирования, математическое моделирования, закон Дарси, визуализация.