Modelling groundwater flow and pollutant transport in hard-rock fractures

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Abstract

There are several reasons for the fact that fracture flow has been a subject of active research for the last three decades. Rock fractures commonly exist in the Earth's upper crust and, therefore, significantly control groundwater movement. Fracture-dominated flow has become increasingly important in various problems of geotechnical interest. A particularly important reason for investigating fracture flow and contaminant transport is the necessity of building repositories of nuclear-fuel waste which are often situated deep in granite massifs. The possibility of their damage during the long periods of storage requires the study of problems connected with the risk of possible contaminant displacement.

The aim of this article is to model water flow and contaminant transport in hard-rock fractures. Such results are required that make it possible to determine the hydraulic parameters of real fractures by comparison with data measurable under field conditions.

Making use of the known hydromechanical characteristics of the modelled fracture and the aqueous phase, a problem with a set of three partial differential equations and related boundary conditions was formulated and numerically solved. The unknown functions of the problem are the liquid-phase pressure, the flow velocity and the contaminant concentration. The method of solution is described and the achieved results are visualized and presented.

1 Introduction

The safety of deep repositories of spent nuclear fuel is a matter of great relevance and importance. In the course of long duration storage, radionuclides can leach out of their containers and spread into the surrounding host-rock materials. Prediction of the rate of contaminants migration will depend on the hydraulic characteristics
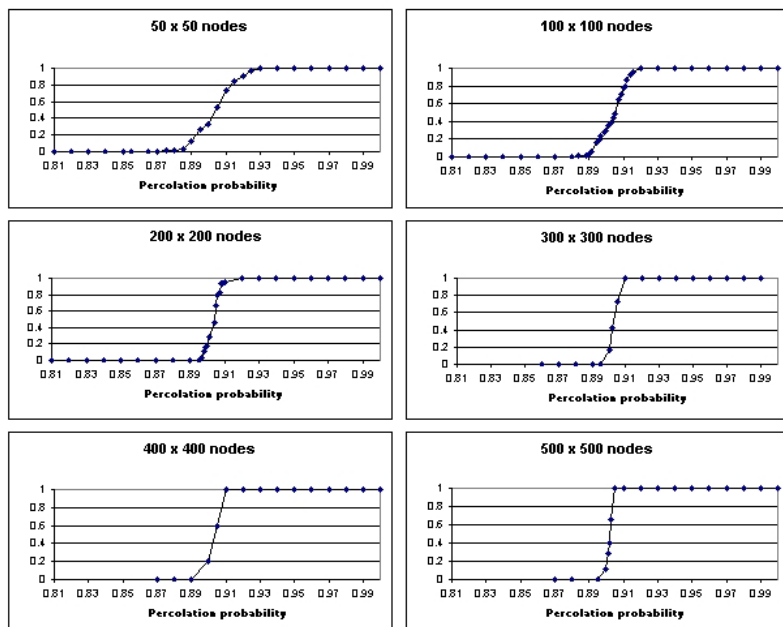
Figure 1: Dependence of probability of permeable fracture on percolation probability for different numbers of sites.

of the fracture system and the sorption characteristics of migrants and the host-rock material.

In order to successfully simulate the fracture flow of the aqueous phase, we need to define the fracture geometry and to find a correspondence between the hydraulic characteristics of the fracture and data measurable in situ.

There are several approaches to the problem of fracture-geometry description. The variable aperture model is the most general one. The model incorporates variable aperture within the fracture space and makes it possible to consider open and closed regions of the fracture. The assignment of the aperture values is usually done by means of geostatistical methods (Moreno et al. [9], Nordqvist et al. [11]). The aperture values are then defined by an aperture probability distribution. Both the normal distribution (Mourzenko et al. [10], Volik et al. [17]) and the lognormal aperture distribution (Nordqvist et al. [11], Ewing and Jaynes [3]) have been used. Another approach to fracture geometry is an application of the percolation theory, e.g. Stauffer and Aharony [15], Berkowitz [2], Renshaw [14]. The percolation theory works with lattices formed of different elements (triangles in the present case) and studies their statistics. For all the latices, each site (triangle) or bond (common boundary of neighboring sites) is randomly occupied (open for aqueous phase) with a given probability p or empty (closed) with probability $1 - p$.

According to the prescribed value p, the resulting fracture becomes permeable or not permeable for the aqueous phase. After that, the proper value of fracture permeability is modelled by means of aperture distribution.

Veselý and Mls [16] studied the influence of the fracture grid size on the relation between the percolation probability p and the probability of the fracture to be permeable. It was found that the increasing number of sites narrows the transition zone of p between the impermeable and the permeable fracture. These results are shown in Figure 1, where the percolation probabilities are depicted horizontally and the probabilities of permeable fractures vertically.

The governing equation of the liquid-phase flow is the continuity equation together with an equation defining the relation between the discharge density and the gradients of pressure and geodetic head. The well known Hagen-Poiseuille equation is generally used for this relation. The resulting equation is usually called the Reynolds equation, e.g. Zimmerman et al. [18]. Ge [4] further extended the Reynolds equation by incorporating tortuosity and the effect of the angle of fracture walls. Konzuk and Kueper [8] pointed out that using locally held Hagen-Poiseuille equation leads to overestimation of the fracture-flow rate by a factor ranging from 1.3 to 1.9.

2 Equations of liquid-phase flow

The liquid-phase flow within the fracture space is governed by two basic laws. The first one is the mass balance equation

$$\sigma \, d(x) \frac{\partial p}{\partial t}(x,t) + \frac{\partial q_i}{\partial x_i}(x,t) = 0 \,, \tag{1}$$

where $x = (x_1, x_2)$ are coordinates in the fracture plane, d is the aperture, σ is specific storage of the fracture, p is the liquid-phase pressure, t is time, and $q = (q_1, q_2)$ is specific discharge of the liquid phase. This equation is accompanied by the Hagen-Poiseuille equation

$$q_i(x,t) = -\frac{d^3(x)}{12 \, \mu} \left(\rho \, g \, \frac{\partial z}{\partial x_i} + \frac{\partial p}{\partial x_i}(x,t) \right) \,, \qquad i = 1, 2, \tag{2}$$

where z is vertically upward oriented coordinate, g is gravity acceleration, and μ is the dynamic viscosity of the liquid phase. Putting these equations together, we obtain second order partial differential equation

$$\sigma \, d(x) \frac{\partial p}{\partial t}(x,t) - \frac{\partial}{\partial x_i} \left(\frac{d^3(x)}{12 \, \mu} \left(\rho \, g \, \frac{\partial z}{\partial x_i} + \frac{\partial p}{\partial x_i}(x,t) \right) \right) = 0 \,, \tag{3}$$

Under the assumption of incompressible liquid phase, Equation (3) simplifies by introducing hydraulic head u,

$$u(x,t) = z(x) + \frac{p(x,t)}{\rho \, g} \,. \tag{4}$$

Assuming further steady-state flow or zero value of specific storativity, Equations (1) and (2) become

$$\frac{\partial q_i}{\partial x_i}(x,t) = 0 \,, \tag{5}$$

$$q_i(x,t) = -\frac{\rho \, g \, d^3(x)}{12 \, \mu} \frac{\partial u}{\partial x_i}(x,t) \,, \qquad i = 1,2. \tag{6}$$

3 Equations of solute transport in fractures

Let us consider a presence of a contaminant in the water within the fracture space. Correct prediction of the contaminant movement depends on several characteristics of the hydrogeological environment (e.g. fracture geometry, discharge density) and the contaminant itself (e.g. solubility, sorptive binding). Denoting c the contaminant concentration (mass of contaminant per volume of the aqueous phase), the transport equation is

$$d(x)\frac{\partial c}{\partial t}(x,t) = \frac{\partial}{\partial x_i}\Big(d(x)\,D\,\frac{\partial c}{\partial x_i}(x,t) - c(x,t)\,q_i(x,t)\Big) - 2\frac{\partial a}{\partial t}(x,t)\,, \quad (7)$$

where D is coefficient of molecular diffusion and a is the mass of the contaminant sorbed on unit surface of the solid phase. In most cases, isotherms of Langmuir and Freundlich are used to asses the effects of the concentration on sorption, e.g. Park and Hahn [12]. The Freundlich isotherm is

$$a = K\,c^n \tag{8}$$

and the Langmuir isotherm is

$$a = \frac{K_1\,c}{K_2\,c + 1}\,, \tag{9}$$

where K, K_1, K_2, n are constants depending on the solid phase and the contaminant in question.

4 Measured data

Measurements of real fracture apertures and asperities are difficult to obtain in practice. It is even more complicated to obtain such data for deep laying fractures. Hence, the inverse modelling is probably the most promising approach to this problem.

Several laboratory measurements were performed and published aimed at getting knowledge of real aperture and asperity sizes, e.g. Pyrak-Nolte et al. [13], Hakami et al. [5], Hakami and Larsson [6]. For crystalline rock, it is possible to conclude that the typical average apertures range from 10 to 600 micrometers. The asperity sizes are in millimeters. According to the laboratory conditions of the measurements, it may be expected that the asperity data are more reliable.

A relatively well described fracture flow experiment was conducted at the Stripa mine in Sweden (Abelin et al. [1]). The experiment took place in a granite massif at the depth of 360 m in several excavated test drifts. Using a large-scale plastic sheeting technique, a very detailed monitoring of water inflow was performed. It was found that the water inflow rates ranged from 0.01 l m^{-1} h^{-1} to 0.06 l m^{-1} h^{-1} with one exception of 0.26 l m^{-1} h^{-1}. The presence of tritium in some locations and its absence in others indicated that there were several isolated channels which led water down to the depth of 360 meters in less than 30 years whereas most of the water had a longer residence time.

The obtained experimental data are of crucial importance when modelling the fracture geometry. The parameters of the fracture generation must be determined in such a way that the computed flow is in agreement with the measured values.

Knowledge of the process of contaminant transport through the real fraction enables us to get further data for the fraction geometry calibration. Under the assumption that the transport parameters of the migrant and the rock material are known, particularly parameters of sorption and molecular diffusion, the fracture geometry can be calibrated by reaching agreement between the measured and computed values of the migrant concentration.

Geologic media may consist of variety of sorbing materials such as micas, iron, silicate or manganese oxides, each with their own sorption preferences for individual solutes and each with different sorption capacity. Park and Hahn [12] investigated sorption and desorption of selected radionuclides on granite. Particularly, the sorptive binding of ^{60}Co, ^{85}Sr and ^{137}Cs on the Bulguksa granite was studied. The obtained results enabled the authors to determine values of the coefficients K, n and K_1, K_2 of Freundlich and Langmuir isotherms (8) and (9). The Langmuir isotherm and the values $K_1 = 5.0 \times 10^{-2}$ m^3/Ci and $K_2 = 4.63 \times 10^{-4}$ m^3/m^2 of ^{137}Cs were used in numerical solutions presented below.

5 The mixed formulation of the flow equation

The transport equation (7) requires values of specific discharge q. Hence, the systems of Equations (5) to (7) or (3), (2) and (7) must be solved in order to obtain required value of concentration $c(x, t)$. If the influence of c values upon the phase density ρ is negligible, Equation (3) can be solved separately and the parameter q can be obtained by means of Equation (2). It is well known that the Rothe method and subsequently the Galerkin method are efficient when solving initial-boundary value problems in Equation (3). Unfortunately, specific discharge obtained in this way does not satisfy the requirements of Equation (7) which is very sensitive namely to this parameter. The flow through individual bonds of the applied lattice (balance between neighbouring elements) has to determined with high level of accuracy. Consequently, it is necessary to reformulate the flow problem in the following way, known as the mixed formulation, e.g. (Kaasschieter and Huijben [7]). Starting with a boundary value problem in Equations (5)

and (6) on a domain Ω, the mixed variational formulation is to find functions $(u, \mathbf{q}) \in L^2(\Omega) \times H^*(div, \Omega)$ such that

$$\int_\Omega \frac{\partial q_i}{\partial x_i}(x)\, \varphi(x)\, \mathrm{d}x = 0 \tag{10}$$

and

$$-\int_\Omega \frac{12\,\mu}{\rho\,g\,d^3(x)}\, q_i(x)\, v_i(x)\, \mathrm{d}x + \int_\Omega u\, \frac{\partial v_i}{\partial x_i}(x)\, \mathrm{d}x = \int_{\Gamma_D} u_D\, v_i\, \nu_i\, \mathrm{d}S \tag{11}$$

$\forall \varphi \in L^2(\Omega)$ and $\forall \mathbf{v} \in H_N(div, \Omega)$, where

$$H^*(div, \Omega) = \left\{ (v_1, v_2); v_1, v_2 \in L^2(\Omega)\,, \frac{\partial v_i}{\partial x_i} \in L^2(\Omega),\ v_i\, \nu_i = q_N \text{ on } \Gamma_N \right\},$$

$$H_N(div, \Omega) = \left\{ (v_1, v_2); v_1, v_2 \in L^2(\Omega)\,, \frac{\partial v_i}{\partial x_i} \in L^2(\Omega),\ v_i\, \nu_i = 0 \text{ on } \Gamma_N \right\},$$

(ν_1, ν_2) is the unit outward normal to Ω, $\partial\Omega = \Gamma_D \cup \Gamma_N$, and $u = u_D$ on Γ_D and $q_i\, \nu_i = q_N$ on Γ_N are the imposed Dirichlet and Neumann boundary conditions on Γ_D and Γ_N, respectively. Using further the Raviart-Thomas finite element formulation and hybridizing the mixed method a system of linear equations is formulated which has symmetric positive-definite matrix, (Kaasschieter and Huijben [6]). The values of specific discharge q obtained in this way satisfy the requirements of the transport equation. Having obtained functions q_1, q_2, initial-boundary value problems in Equation (7) can be solved by means of the Rothe method.

6 Numerical solution

A fracture was generated using the above method based on the percolation theory approach. Making use of the defined fracture parameters, several flow problems were numerically solved. For the obtained specific discharge values, several transport problems were solved separately. S-curves were modelled by imposing proper initial and boundary conditions. The reason for this choice was that s-curves reflect the most common tracer experiments. Different values of the flow rate were obtained by changing the slope of the fracture. Fig. 2 shows the response: s-curves 1, 2, and 3 were obtained for the same fracture and for slopes of $\pi/3$, $\pi/4$ and $\pi/6$, respectively.

The influence of concentration and aperture values on the sorption process is shown in Figure 3. Two different values of mean aperture (5×10^{-5} and 5×10^{-4}) and two different values of concentration (0.2 Ci/m^3 and 1.5 Ci/m^3) were chosen and the computations were carried out for their combinations. The differences between the resulting s-curves demonstrate the sensitivity. Curves 2 and 4 were obtained with the lower asperity. The specific discharge was kept unchanged.
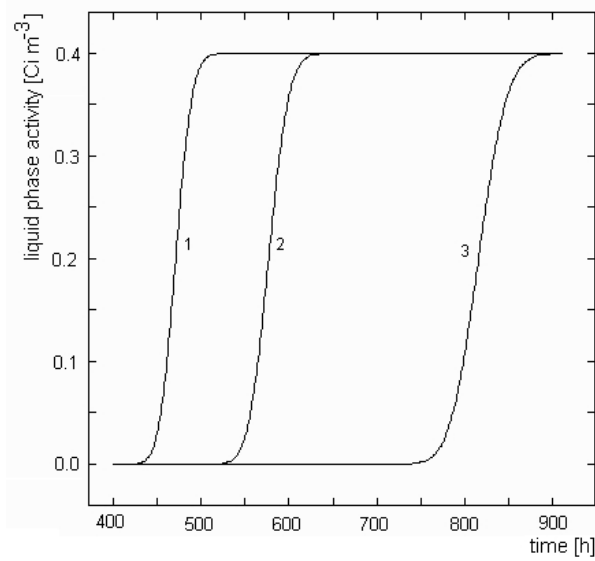
Figure 2: Dependence of the outflow concentration on time for three different values of specific discharge.
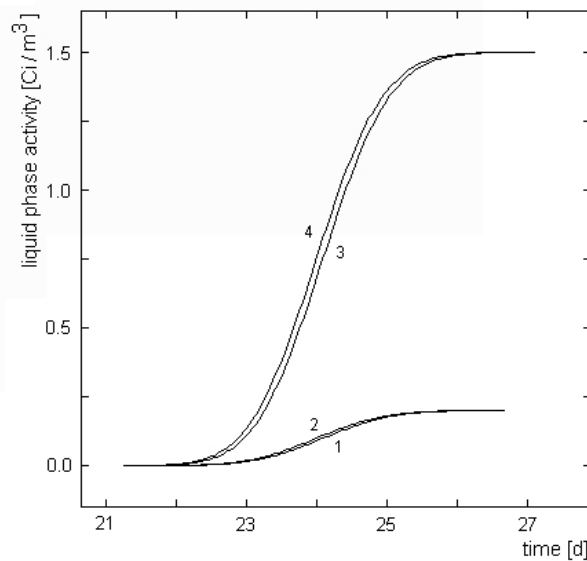

Figure 3: Dependence of the outflow concentration on time for different values of aperture and inflow concentration.

Acknowledgements

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