Flow Lab. : Flow Visualization and Simulation
핵종이동 가시적 현상관찰및 수치모사

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Abstract

The experimental setups for flow visualization and processes identification in laboratory scale (so called Flow Lab.) has developed to get ideas and answer fundamental questions of flow and migration in geologic media. The setup was made of a granite block of 50x50*cm* scale and a transparent acrylate plate. The tracers used in this experiments were tritiated water, anions, and sorbing cations as well as an organic dye, eosine, to visualize migration paths. The migration plumes were taken with a digital camera as a function of time and stored as digital images. A migration model was also developed to describe and identify the transport processes. Computer simulation was carried out not only for the hydraulic behavior such as distributions of pressure and flow vectors in the fracture but also for the migration plume and the elution curves.

Key word : flow lab. migration plume, fracture, visualization, sorption, matrix diffusion

요 약

지하매질에서 핵종이동현상을 가시적으로 관찰할 수 있는 실험실규모 실험장치를 개발하여 이동실험을 수행하였다. 이 실험장치는 50x50cm 규모 화강암과 아크릴상층부로 구성되어있다. 실험에는 삼중수소, 음이온, 수착성양이온뿐 만 아니라 이동경로를 관찰할 수 있는 유기염료도 포함하였다. 시간에 따른 물질이동양태를 사진을 찍어 컴퓨터에 저장하였다. 또, 이동과정을 모사하고 단위공정별로 분석해 볼 수 잇는 이동모델도 개발하였다. 컴퓨터모사를 통해 균열내 흐름장에서 압력과 유속분포를 계산하고, 균열내 이동양태와 유출곡선을 계산해 실험결과와 비교평가하였다.

중심단어 : 이동양태, 균열, 가시화, 수착, 매질내 확산,

1. Introduction

The transport processes of contaminants in the geologic media can not be observed directly like a black box. Only we can check the output from the transport. However, if there is an idea to see the internal phenomena in the black box, it will be very helpful to analyze the process and build a model. The first flow visualization and processes laboratory was developed by Sandia National Laboratory, USA in early 1990s[1]. And it was named "Flow Lab.". In Korea, a kind of flow lab. has developed from late 1990s by KAERI[2]. Transparent fractures can be used to study various flow processes in the environmental field. Transparent fractures can be designed and fabricated with varying aperture in a range of probable structures or be cast from individual natural fractures in epoxy or glass to yield a realization of nature. Similarly, we used an acrylate plate to simulate the fracture system for the observation of migration plumes of organic dye in the fracture. Such visible images of migration plume in the analog fracture may give important suggestions and informations in understanding the invisible migration plum in the rock fracture. Fractures in rocks tend to dominate the hydraulic behavior, particularly when the rock matrix is of low permeability. Individual fractures act as conduits through the media and allow free passage between the matrix blocks which bound the fracture.

In this study, we are focused on physicochemical interactions between rock and chemical species. Thus, we designed a simple fracture system having a pair of parallel plates. In order to describe the fluid flow in the fractured rock, we make the assumption that each fracture is idealized as a pair of parallel plates separated by a constant distance which represents the aperture of the fracture. The processes to be considered are advection, dispersion, and sorption in the fracture plane, coupled with diffusion of the tracer into the stagnant pores in the rock matrix. These last two processes can be significant processes for retarding the migration of tracers. Thus diffusion into the rock mass in the fracture surface was treated as an important study topic in this experiment. For this work, we were compared migration characteristics of tracers according to their chemical properties ; water, anion, sorbing cation, and polymers. We are also going to develop a generic model describing the migration of the tracers in various rock fractures, that is, to develop a variable aperture channel model for characterizing the fracture plane including a constant aperture fracture. And a particle tracking scheme is applied for the solute transport. We will present our investigations of the flow and migration in two-dimensions, representing the physical situation of the experimental setup.

2. Transport Model

The fracture plane may be subdivided into imaginary subsquares. The fluid flow through the fracture is then calculated for a constant injection/withdrawal rate as well as for constant pressure conditions. For a constant laminar flow, the volumetric flow rate through a parallel fracture may be written as:

$$Q = \frac{1}{12\,\mu}\,\frac{b^3\,W}{L}\,\Delta P \qquad (1)$$

where ΔP is the pressure drop over a length of L and W and μ is the viscosity. Eq.(1) may be applied to each of the subsquares enclosed by the grid lines. When the volumetric flow rate from node i to node j is Q_{ij} , the volumetric flow rate can be rewritten

$$\sum_j Q_{ij} = \sum_j C_{ij} (P_i - P_j) = E_i \qquad (2)$$

where E_i is the injection rate or withdrawal rate at node i. The subscript j stands for the four facing nodes of surrounding subsquares to node i.

Except for the nodes at the boundaries, the pressure at each node is unknown to be solved with the Gauss-Seidel iteration method. The flow between adjacent nodes can be calculated using eq.(2). After obtaining flow vectors at all nodes, solute transport can be simulated in this flow field.

A two-dimensional random-walk particle tracking algorithm is used to simulate the solute transport through the flow fields. Particle displacements in each time step consisted of an advective displacement based on local velocities calculated using the pressure field and random diffusive displacement. Particles, which are representing the mass of a solute contained in a defined volume of fluid, move through a fracture with two types of motion. One motion is with the mean flow along stream lines and the other is random motion, governed by scaled probability.

At the inlet, a certain amount of particles were introduced, and distributed at each node between flow channels with a probability proportional to the flow rates. Particles are then convected by discrete steps from node to node until they reach the outlet node at which point the arrival time is recorded. This procedure is repeated for all of particles to get a stable probability distribution. The residence time for nonsorbing tracers in a given subsquare is determined from the total flow through that subsquare and its volume. The residence time of a particle along each path is obtained as the sum of the residence times in all subsquares through which the particle had passed. Four transport processes are considered in modelling the solute transport: advection(V), hydrodynamic dispersion(D_s), diffusion into the rock mass(D_e), and sorption(K_a).

3. Experimental

A block of Hwangdeung granite with dimensions of 50x50x10(*cm*) containing an artificial open fracture was prepared. The rock has a little amount of secondary minerals : It means that this rock is a little weathered. Also this rock has an interconnected porosity of 0.37 % with the specific gravity of 2.55.

The experimental setup having dimensions of 50x50x10(*cm*) was prepared. The setup is designed for taking the images of the migration plume and this analog fracture is fabricated by holding an **acrylate** as the upper plate and granite as the lower one in close contact. When a tracer migrates through the gap between the acrylate and the granite, the migration plume can be observed through the transparent acrylate plate. The setup was assembled by placing the fracture plates in contact and bolting the frames together to a uniform torque. The outer gap of the fracture was sealed with a silicone adhesive to prevent from leaking of fluid. Stainless steel frames were mounted on both halves of the block and connected to each other by four threaded rods and bolts. Two boreholes on the upper plate are selected as the inlet and the outlet for transporting of fluid. Before the migration test, gases in the rock fracture were evacuated and the rock block was submerged in the water container to be saturated with water. The water in the container has kept almost a constant temperature of 20°C.

Four kinds of chemical species were used for migration test ; (1) tritiated water(*THO*), (2) anion ; Cl^- & Br^-, (3)polymeric organic dye ; *NaLS* (sodium lignosulfonate, M_w=24,000) and Eosine ($C_{20}H_6Br_4Na_2O_5$, M_w=691) , and (4) sorbing cation ; Sr^{+2} & Cu^{+2}. The aliquot solution of 1.2 *ml* containing tracers was injected as a band input function into the inlet borehole in separate campaigns, fed with a HPLC pump through the fracture at a flow rate of 0.5 *ml/min* and collected at the outlet borehole as shown in Fig.1. The eluted solution was collected using a fraction collector.

The flow was directed along the gap of the fracture through implementation of no-flow boundaries along the fracture sides. The fluid was uniformly supplied to the inlet hole using a HPLC pump, creating a constant flow boundary condition. At the downstream end of the fracture, a constant head boundary was implemented. Especially, Eosine, an organic dye, was used to visualize the migration

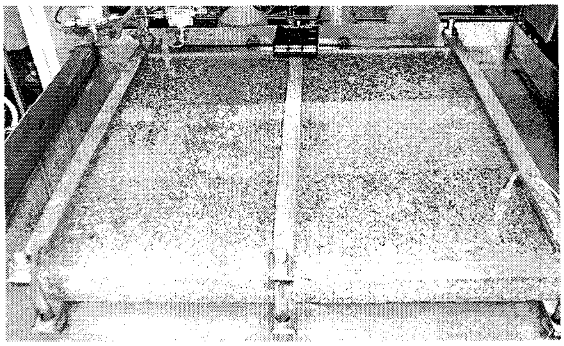


Fig.1 The Experimental setup for the migration test

Transparent Fracture Analoge, upper plate : acrylate, bottom plate : granite [50x50x5.5(cm)] plume in the flow plane of the setup1. The migration plumes were taken with a digital camera as a function of time and stored as a digital image file.

The concentrations of eosine and *NaLS* were analysed with the UV/VIS spectrophotometer at the wavelength of 524*nm*, 282*nm*, respectively. The concentrations of Cl^- and Br^- were analysed with the ion electrodes of Orion Research Inc.. Sr^{+2} and Cu^{+2} were analysed with the ICP-MS. *THO* was analysed with a Liquid Scintillation Counter.

4. Simulation of Hydraulic Properties and Migration in the Fracture

The fracture surface was divided into an imaginary matrix of 20x20 sub-squares. All sub-squares were assigned the same aperture value. Recall that the boundary conditions employed to solve the flow through the system are the constant head boundary condition ; that is, injection node is at the higher constant pressure P_1 and the withdrawal node is at the lower constant pressure P_2. The flow between adjacent nodes can be calculated using Eq.(2). The pressure distribution in the field was simulated with a graphic program SURFER as shown in Fig.2. The pressure drop, ΔP, between the inlet and the outlet were about $280 N/m^2$ in the setup. Then the aperture could be calculated with the ΔP and eq.(1). The difference of pressure drop between two setups is probably due to the differences of aperture size and the viscosity of media.

Fig.3 showed two dimensional flow field and some examples of supposable stream traces, which was plotted with a commercial program TECPLOT. Figs.2 and 3 showed symmetric trends in the distributions of the pressure and the flow vector pivoting the diagonal line between the inlet and the outlet. At the edges of both sides of the fracture, the flow vectors were very small, and thus the flow was regarded as almost

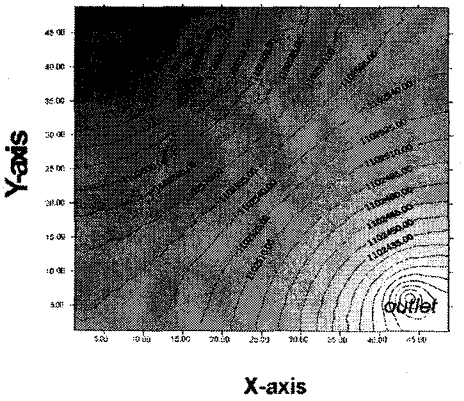


Fig.2 Simulation result of Pressure distribution in the fracture

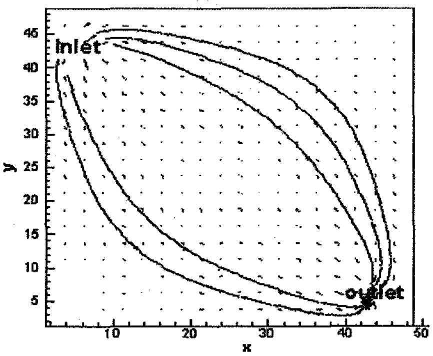


Fig.3 Distribution of flow vectors in flow field and some examples of stream tracers

The migration plume of the organic dye, eosine, in the setup was taken with a digital camera as a function of time and shown in Fig.4. The migration plume did not follow a linear trace along the diagonal direction between the inlet and the outlet, but moved across the full width of the fracture as a two dimensional span around the diagonal line. Thus a two dimensional migration model is required to describe this migration plume and, needless to say, it is difficult to apply one dimensional model. Comparing this results with the simulated one in Fig.5, the general trend was consistent with each other. In this simulation, matrix diffusion of eosine in both fracture sides was ignored. Though the simulated migration plume showed perfect symmetric fan-shape around the diagonal line, the experimental one did not show symmetric shape at later stage. It seems to be due to the discrepancy between experimental setup and model assumption of the constant aperture. Near the outlet of the setup there might be some variation of aperture value and showed irregular shape of migration plume at later stage. Because the flow is proportional to the cube of the aperture, even the smallest change of the aperture can give large effect on the migration plume.

5. The Elution Curve and Retardation

The simulated and experimental elution curves of the tracer were shown together in Fig.6. The simulated curves were obtained from the residence times of the 10,000 particles through the fracture. When advection, sorption, hydrodynamic dispersion and diffusion into the rock mass are considered, different particles in the same subsquare will have different residence times. The residence times for these particles can be expressed as a probability density function which in turn can be regarded as the elution concentration of a pulse injection. Integrating this curve over time gives a cumulative elution profile as shown in Fig.7. In general, the cummulative elution curves of tracer transport in two dimensions through those flow field have a fast rise at early times, since the majority of particles take the fastest flow paths; then there is a long tail in the breakthrough curve due to a small fraction of particles meandering through the fracture with small volumetric flow rates.

The calculated aperture value, b, was 0.016*cm*. It gives resonable correspondence with the simulated result of 0.011cm using the pressure difference of 280N/m^2 between the inlet and the outlet as shown in Fig.3. While linear velocity in the fracture is expressed as,

$$u = Q/(W \cdot b) \qquad (3)$$

The obtained value of u is 0.63 *cm/min*. In Fig.6, residence time of nonsorbing tracer in the fracture are approximately 80 minutes, or as eluted volume, 40 *ml*. If the tracer follow a linear trace along the diagonal line of 43 *cm* long between the inlet and the outlet, then the aperture should be larger than 0.1*cm* to get the travel time about 80 min. ; that would be unreasonably large value of the aperture. Therefore, the tracer did not across the straight line of the shortest course, but move as a two dimensional fan-shape as shown in Fig.4. To analyze the migration characteristics of tracers according to their chemical properties, the elution curves and the cummulative elution curves were examined in Figs.6 & 7. In these curves, the tritiated water was regarded as a basic tracer because it has same chemical properties with the water. Usually, tritium, anion, and some organic dye are assumed as the nonsorbing tracer. Therefore, in modeling work, it is commonly assumed that the distribution coefficient, $Ka=0$, and the retardation factor, $R=1$, for such nonsorbing tracers. However, in this experiment, They showed different migration behavior. The anions and polymeric organic dyes migrate faster than the tritium in the natural fracture and they are recovered almost 100% at the exit. While tritium was recovered only 83%. This phenomenum can be explained in two aspects. First, because the surface of the rock fracture is negatively charged, the anion could be expelled by the rock surface and thus can not access to the pore by the anion exclusion effect. Second, the ionic size of the polymeric organic dye is larger than cations by over 1000 times. And the size of the micropores of the rock ranges from micrometer to subnanometer. Considering that the ionic size of the cation is about several Å, cations and water molecule can penetrate easily into the micropore of the rock, while the polymeric substances can not. Therefore, it could be concluded that tritium diffuses into the rock pores, but anions and polymeric tracers hardly diffuse into the rock matrix. The migrating sorbing tracer interacts with the fracture surface and it retards as much as their sorption capacity. The degree of retardation is usually expressed as the retardation factor, R

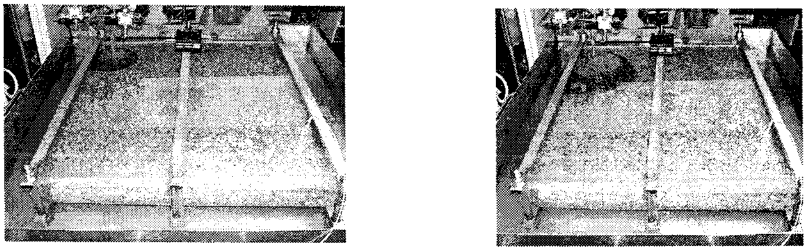
$$R = \frac{\tau_n}{\tau_w} = \frac{u_w}{u_n} = 1 + \frac{K_a}{b} \qquad (4)$$

where, τ_n : tracer travel time, τ_w : water travel time, u_w : water velocity , u_n : tracer migration velocity.

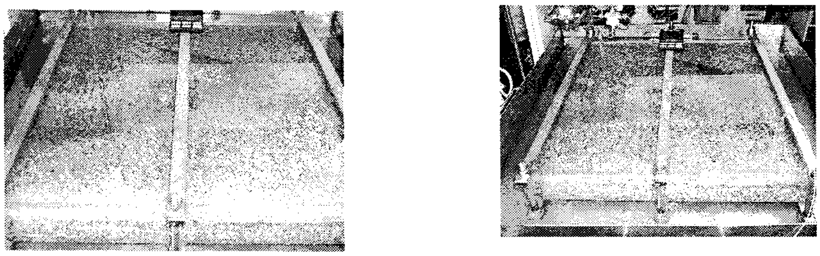
The R values from the elution curve was smaller than the R values from the sorption data. It seems that the sorbing tracers did not interact sufficiently with the rock surface in the flow rate of *0.5 ml/min.*

6. Conclusion

The flow visualization and processes identification has been carried out successfully using the experimental setup, a kind of "Flow Lab.". The migration plume through fracture taken with a digital camera corresponded to the results of model simulation reasonably. The tracers moved as two dimensional span rather than one-dimensional straight line course between the inlet and the outlet in this fracture system. The combination of the experimental observation and the model simulation gave good suggestions to further understand the flow and transport in the rock fracture.

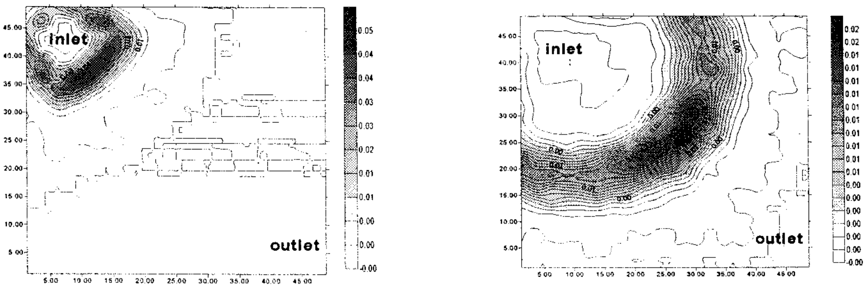


(a) 20 min. (b) 40 min.

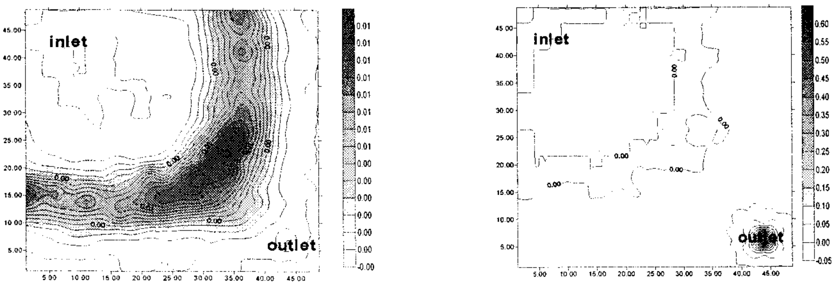


(c) 60 min. (d) 80 min.

Fig. 4 Migration plume of eosine in the analoge fracture as a function of time



(a) 20 min (b) 40 min



(c) 60 min (d) 80 min

Fig. 5 Simulated Contours of Migration Plume in the Fracture with time

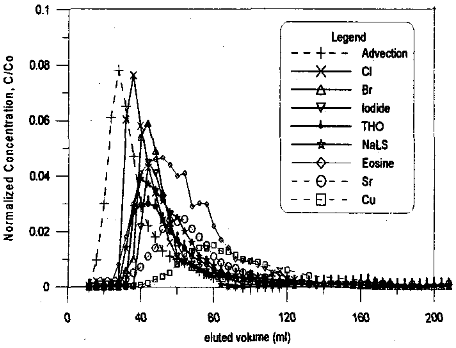


Fig.6 Simulated and Experimental Elution Curves

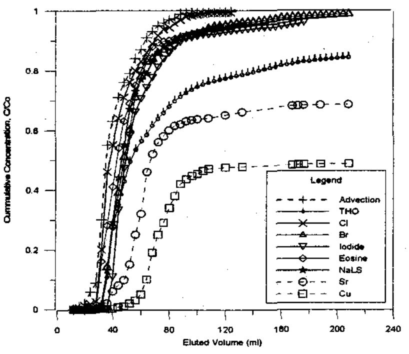


Fig.7 Simulated and Experimental Cumulative Curves

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