Simulation of Radionuclide Transport in the Engineered Barrier System of a Geological Repository

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1. Introduction

After closure of the geological repository, the coupled thermal, hydrological and mechanical processes such as the heat generation from a waste, the intrusion of groundwater from a surrounding rock, and the stress changes due to the swelling of a buffer will be occurred in the engineered barrier system. The thermal gradient in a buffer due to decay heat can accelerate the migration of radionuclides through the buffer, and the drying and resaturation processes occurring in the buffer may have a critical impact on the release of radionuclides from the disposed waste. In investigating the migration of ions and contaminants in a porous medium, a saturated condition has been commonly assumed, and several works [1-3] have considered the transport of ions in an unsaturated porous medium. However, the migration of radionuclides through a partially saturated medium with a thermal gradient has not been fully studied.

In this study, the simulation results of the coupled thermal, hydrological, and chemical processes occurring in the engineered barrier system of a geological repository using the TOUGH2 computer code [4] are presented.

2. Mathematical Model

TOUGH2 [4] is a general-purpose numerical simulation program for multi-dimensional fluid and heat flows of a multiphase, multicomponent fluid mixture in an unsaturated medium.

Fluid advection is described with a multiphase extension of Darcy' law. Heat accumulation and heat flux are

$$\begin{split} M^{\text{heat}} &= (1-\emptyset) \; \rho_{\text{s}} \; C_{\text{s}} \, T + \; \emptyset \; \sum_{\beta} S_{\beta} \; \rho_{\beta} \; u_{\beta} \end{split}$$

$$F^{\text{heat}} &= -\lambda_t \; \nabla T + \; \sum_{\beta} \; h_{\beta} \; F_{\beta} \end{split}$$

where C, u, λ_t and h are the specific heat, specific internal energy, thermal conductivity and specific enthalphy, respectively. The subscript *s* expresses a solid medium. The radionuclide transport through a medium is assumed to occur by diffusion. The dependency of diffusion coefficients for gas components on the pressure and temperature is considered in the model. But aqueous diffusion coefficients are taken as constants because there is not a significant difference under the simulation condition. Adsorption of radionuclides on the bentonite is modeled as reversible instantaneous linear sorption and the radionuclide partition between aqueous and gaseous phases is described by Henry's law. Radionuclides are assumed to be decayed by the first-order decay

3. Simulation

The temperature, moisture and radionuclide concentration distributions in the bentonite buffer of KENTEX-C were analyzed using the presented model.

The KENTEX-C is a modified version of KENTEX (KAERI Engineering-scale THM Experiment for an Engineered Barrier System) which is an experimental facility to study the THM behavior in an engineered barrier system at KAERI in Korea [5]. KENTEX-C is to investigate the transport of ions through a partially saturated buffer with a thermal gradient.

The detailed geometry of KENTEX-C was incorporated into the model. The configuration of KENTEX-C was modeled with a two-dimensional radially-symmetric mesh, for representing a cylindrical heater emplaced in the compacted bentonite buffer in a steel confining cylinder

3.1. Material Parameters

To measure the diffusion coefficients in compacted saturated bentonite with a dry density of 1.5 Mg/m³, the "in-diffusion" method was used. After the diffusion period, the bentonite plug was sectioned into slices 2 mm thick. The slice was extracted using a 1 M HCl solution and after centrifuging and filtering, the solution was analyzed for Γ and Cs⁺ by an ion selective electrode meter and ion chromatography, respectively. The concentration profile for Cs⁺ in the bentonite plug after the diffusion coefficients obtained from the concentration profiles are 2.95×10^{-10} m²/s for Γ and 2.18×10^{-11} m²/s for Cs⁺, respectively

The hydraulic conductivities were found to decrease with an increase in the dry density of the bentonite. The relation between the logarithm of the hydraulic conductivity, K (m/s) and the dry density of the bentonite, ρ_d (Mg/m³), can be fitted to a straight line expressed as follows :

$$\log K = -4.07 \rho_d - 6.13$$
 $r^2 = 0.92$

The two-phase relative permeability was described using the Grant correlation .



Fig. 1. Concentration profile for Cs^+ in the bentonite plug after diffusion time

3.2. Simulation Results

The calculated time-dependent concentrations versus the distance from the heater surface for iodide and cesium are shown in Fig. 2 and Fig. 3. The ion concentration in the buffer is expressed as the normalized concentration defined as C/C₀, where C₀ is the initial bulk concentration of the ion in the bentonite at the hydration surface. The concentration of ion in the bentonite buffer increases with time progressively due to the diffusion from the wall of the confining cylinder. I⁻ diffused fast through the bentonite buffer, and its high diffusion rate is attributed to the fact that I as a monovalent anion was not sorbed on the bentonite. On the other hand, Cs⁺ which is an uncomplexed monovalent cation is sorbed to a greater extent on the bentonite. The increase of distribution coefficient decreases the apparent diffusion coefficient, which leads the slow diffusion of Cs⁺ through the bentonite pore water.



Fig. 2. Time dependent change of Γ concentration at a height of 0.61 m

3. Conclusions

To simulate the radionuclide migration in the engineered barrier system of geological repository, the

numerical model using TOUGH2 computer code was developed, and applied to analyze the THC behavior of KENTEX-C. The presented model can simulate the coupled thermal, hydrological and chemical process occurred in the engineered barrier system after the closure of the repository. This model can be applied to assess the long-term performance of geological repository. It is also useful for optimizing the design of the engineered barrier system of the repository.



Fig. 3. Time dependent change of $Cs^{\scriptscriptstyle +}$ concentration at a height of 0.61 m

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