

## Reactive Transport of Nuclide in the Presence of Bacteria in the Fractured Rock: Model Development and Verification

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### 1. Introduction

Deep geological disposal of high-level radioactive waste (HLW) for the safe isolation from the biosphere should be accompanied by the understanding of radionuclide transport characteristics and prediction of the long-term radionuclide migration through the fractured rock matrix. The radionuclides leaking from the repository can reach the biosphere through the fracture network of the base rock which is considered as a natural barrier of the repository. The migrating radionuclides interact with rock medium, fracture-filling minerals, and various colloidal, organic, and microbial materials [1]. In addition, the transport of radionuclides can be retarded by the rock matrix diffusion [2].

Because of the deep location (several hundred meters from the ground surface) of the repository and the extremely long time scale (several million to billion years of half life) of radionuclide migration, the accessibility and the reproducibility for the researchers are strongly limited. Therefore, many researches on the mathematical and stochastic modeling have been conducted to predict the behaviors of radionuclides in the deep geological environments and thus to decrease their uncertainty [3]. In this study, accordingly, a numerical model was newly developed to include chemical and biological kinetics in reactive transport of radionuclides in the presence of bacteria in the fractured rock using an operator splitting method. The model was preliminarily verified by comparing with an analytical solution in a simplified condition.

### 2. Methods and Results

#### 2.1 Conceptual Model

Transport of nuclide in the presence of bacteria in the fractured rock is conceptualized in Fig. 1. In addition to the bacteria and nuclide transports, bacteria-facilitated transport of nuclide (FBL in Fig. 1), bacteria growth and decay rates ( $\sum Q^g$  and  $\sum Q_d$ ), microbial utilization rates of nuclide ( $\sum Q_u$ ), bacteria and nuclide adsorption/desorption rates ( $\sum Q_s^f$ ,  $\sum Q_{fb}^f$ ,  $\sum Q_{sb}^f$ ,  $\sum Q_f^s$ ,  $\sum Q_f^{fb}$ , and  $\sum Q_f^{sb}$ ), and nuclide diffusion rates into the rock matrix ( $\sum Q_p^f$ ) were considered in this study. Considering the bacteria size which is several  $\mu\text{m}$  and the high density (or small porosity) of the rock matrix,

only nuclide was assumed to be able to transport through the rock matrix.

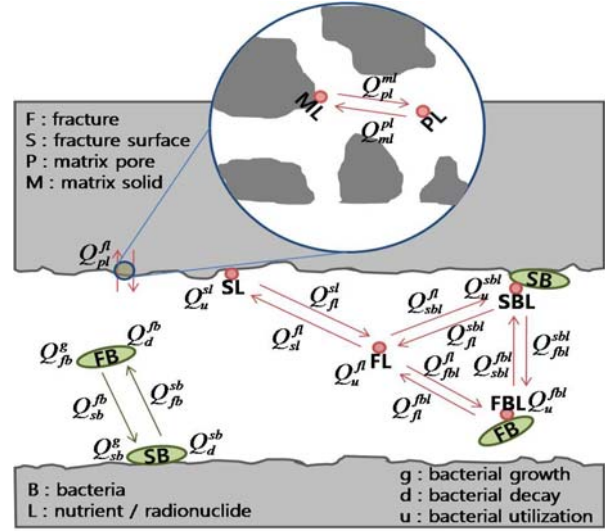


Fig. 1. Schematic of conceptual model of nuclide transport in the presence of bacteria in the fractured rock.

#### 2.2 Governing Equations

The coupled one-dimensional bacteria and nuclide transports in the fracture and in the rock matrix are governed by the following partial differential equations:

$$\frac{\partial F_b}{\partial t} = -v \frac{\partial F_b}{\partial z} + D_{fb} \frac{\partial^2 F_b}{\partial z^2} - Q_{sb}^{fb} + Q_{fb}^{sb} + Q_{fb}^g - Q_d^{fb} \quad (1)$$

$$\frac{\partial F_l}{\partial t} = -v \frac{\partial F_l}{\partial z} + D_{fl} \frac{\partial^2 F_l}{\partial z^2} - Q_{sl}^{fl} + Q_{fl}^{sl} - Q_{fb}^{fl} + Q_{fl}^{fb} - Q_{sb}^{fl} + Q_{fl}^{sb} - Q_{pl}^{fl} - Q_u^{fl} - Q_d^{fl} \quad (2)$$

$$\frac{\partial \sigma_l^{fb} \rho_b V_b F_b}{\partial t} = -v \frac{\partial \sigma_l^{fb} \rho_b V_b F_b}{\partial z} + D_{fb} \frac{\partial^2 \sigma_l^{fb} \rho_b V_b F_b}{\partial z^2} + Q_{fb}^{fl} - Q_{fl}^{fb} - Q_{sb}^{fb} + Q_{fb}^{sb} - Q_u^{fb} - Q_d^{fb} \quad (3)$$

$$\frac{\partial P_l}{\partial t} = D_{pl} \frac{\partial^2 P_l}{\partial x^2} - Q_{ml}^{pl} + Q_{pl}^{ml} - Q_d^{pl} \quad (4)$$

where  $F_b$  and  $F_l$  are the mobile bacteria and nuclide concentrations, respectively, in the fracture,  $\sigma_l^{fb}$  is the mass fraction of nuclides attached on the bacteria and  $P_l$  is the mobile nuclide concentration in the matrix. The mass transfer rate of nuclide by diffusion into the rock matrix ( $\sum Q_p^f$ ) can be expressed by Fick's first law as:

$$Q_m^f = -\frac{\theta \cdot D_{pl}}{b} \frac{\partial P_l}{\partial x} \Big|_{x=b} \quad (5)$$

where  $\theta$  is the porosity of the rock matrix and  $b$  is the half aperture of the fracture. Bacteria growth rates were

explained by multiple Monod equations [4] and other mass transfer rates ( $Q$ ) were explained by the first-order kinetic equations.

For the initial and boundary conditions, it was assumed that the domain had initially no nuclide concentration, and constant concentration at the inlet and no-gradient concentration at the outlet were assumed.

### 2.3 Numerical Analysis

From the kinetics of bacteria and nuclides ( $\sum Q$ ), the governing equations of the bacteria and nuclide transports in the fractured rock (Eqs. (1)-(4)) become nonlinear which are difficult to be solved analytically if it is not impossible. The non-linear governing equations were numerically analyzed by Strang-splitting sequential non-iterative scheme [5] in which the transport terms were separated from the kinetic terms and computed by the fully implicit finite difference method. The linear system by excluding kinetic terms was directly solved by matrix computation using intrinsic MATLAB function.

The overall numerical computation sequences are as follows:

- 1) Compute  $F_b$ ,  $F_l$ ,  $\sigma_l^{fb}$ , and  $P_l$  from the transport terms of Eqs. (1)-(4) for the first half of the time interval ( $dt/2$ ),
- 2) Compute all  $Q$  for the time interval ( $dt$ ),
- 3) Compute  $F_b$ ,  $F_l$ ,  $\sigma_l^{fb}$ , and  $P_l$  from the transport terms of Eqs. (1)-(4) for the last half of the time interval ( $dt/2$ ).

### 2.4 Model Verification

For the verification of the newly developed numerical model, a general analytical solution of the contaminant transport in the fractured rock [6] was employed. The analytical solution dealt with advection, hydrodynamic dispersion in the fracture, radioactive decay, rock matrix diffusion expressed by Fick's first law, and contaminant adsorption onto the fracture surface and within the matrix governed by a linear equilibrium isotherm.

For the model simulation, half of the artificial rock core including a single flat fracture was regarded as a model domain. The domain size was 0.2 m (along the fracture,  $Z$ )  $\times$  0.01 m (toward the matrix,  $X$ ), and the unit width to the  $y$ -axis was 0.052 m ( $Y$ ). As the coupled one-dimensional model, only  $z$ - and  $x$ -axis were discretized. The regular grid spacing of both  $\Delta z$  and  $\Delta x$  was set as 0.0005 m which is equal to the half of fracture aperture.

Figure 2 shows the comparisons between modeling results and relevant analytical solutions depending on the flowrate ( $q$ ). The modeling results of both spatial and temporal distributions in the fracture were well matched with their analytical solutions (Figs. 2(A) and 2(C)). However, the modeling results in the matrix were

slightly overestimated comparing to their analytical solutions (Fig. 2(B)). The errors are presumed to be occurred due to the sudden decrease of nuclide concentration at the interface between fracture and rock matrix.

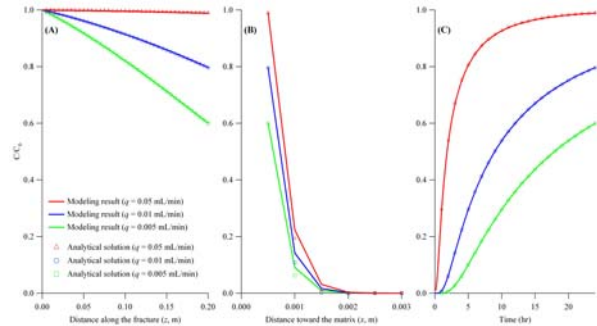


Fig. 2. Comparisons of modeling results with relevant analytical solutions for the spatial distributions along the fracture (A) and toward the matrix at  $z = 0.2$  m (B) after 24 hours and for the temporal distribution at  $z = 0.2$  m (C) depending on the flowrate ( $q$ ).

### 3. Conclusions

The numerical model for the nuclide transport in the presence of bacteria in the fractured rock was developed and, for the preliminary study, the nuclide transport of the model was well verified using the analytical solution. For the further work, the model will be examined for the complex biogeochemical reaction mechanisms in the radionuclide transport and validated by the results of parallel laboratory transport experiments along using rock core column.

### REFERENCES

- [1] M. H. Baik, S. Y. Lee, J. K. Lee, S. S. Kim, C. K. Park, and J. W. Choi, Review and compilation of data on radionuclide migration and retardation for the performance assessment of a HLW repository in Korea, Nuclear Engineering Technology, Vol. 40(7), p. 63-76, 2008.
- [2] P. Holttä, A. Poteri, M. Siitari-Kauppi, and N. Huittinen, Retardation of mobile radionuclides in granitic rock fractures by matrix diffusion, Physics and Chemistry of the Earth, Vol. 33, p. 983-990, 2008.
- [3] K. T. B. MacQuarrie and K. U. Mayer, Reactive transport modeling in fractured rock: A state-of-the-science review, Earth-Science Reviews, Vol. 72, p. 189-227, 2005.
- [4] J. Luo, F.-A. Weber, O. A. Cirpka, W.-M. Wu, J. L. Nyman, J. Carley, P. M. Jardine, C. S. Criddle, P. K. Kitanidis, Modeling in-situ uranium(VI) bioreduction by sulfate-reducing bacteria, Journal of Contaminant Hydrology, Vol. 92, p. 129-148, 2007.
- [5] J. Carayrou, R. Mose, and P. Behra, Operator-splitting procedures for reactive transport and comparison of mass balance errors, Journal of Contaminant Hydrology, Vol. 68, p. 239-268, 2004.
- [6] D. H. Tang, E. O. Frind, E. A. Sudicky, Contaminant transport in fractured porous media: Analytical solution for a single fracture, Water Resources Research, Vol. 17(3), p. 555-564, 1981.