Numerical Simulation on the Diffusion and Sorption of Radionuclides Along the Heterogeneous Microstructures in Rock Matrix

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1. Introduction

The SKB Task Force is a forum for the international organizations supporting the Äspö Hard Rock Laboratory (HRL), Sweden, to interact in the area of conceptual and numerical modelling of groundwater flow and solute transport in fractured rock. The 9th task of this forum was intended to increase realism in solute transport modelling on the in-situ experiments performed at the Äspö HRL (LTDE-SD) and the ONKALO underground rock characterization facility in Finland (REPRO). For the 2nd step of this task (Task 9B), particularly, the inverse modelling have been carried out to characterize the matrix diffusion and sorption of radionuclides in the crystalline rock based on the LTDE-SD experimental results.

2. LTDE-SD and Task 9B

2.1 Summary of the LTDE-SD test

Understanding of matrix diffusion and sorption of radionuclides in the crystalline rock is important in safety assessments for geological disposal of radioactive waste [1]. For this, the LTDE-SD test was performed in a borehole installed at the Äspö HRL during 198 days. The experimental section is surrounded by Ävrö granodiorite and includes a natural fracture at the end of the borehole. Within the section, both of the fracture surface and the wall of slimhole, drilled in the inner rock, were exposed to the cocktail mixed with 22 radioactive tracers (Fig. 1). After the termination, the rock surrounding the borehole was overcored and then small core samples were drilled axially (A-core) from the fracture surface section and radially (D-core) from the slimhole section (Fig. 1). The surfaces of A-cores have fracture coating and alteration while the surfaces of D-cores might include damaged zone created from the drilling process of slimhole.

One of the main results from the LTDE-SD test must be the penetration profile of ^{137}Cs having two slopes. In the profile, particularly, the flat slope of tailing part might imply the tracers reaching much longer into the rock matrix than that expected from a homogeneous diffusion/sorption model [2]. The primary objective of Task 9B was to interpret and understand this anomalous result of LTDE-SD test through more realistic modelling work.

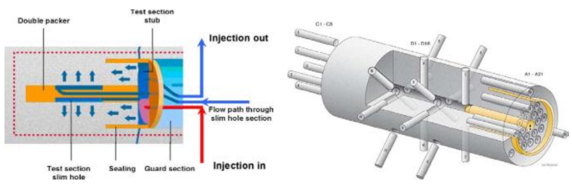

Fig. 1. The schematic diagrams of LTDE-SD experimental section (left) and overcored rock (right) [2].

2.2 Modelling approach in this study

In microscopic scale, open and sealed micropores along mineral grain boundaries or inside mineral grains are observed in rock. Particularly, well-connected micropores could act as a potential path of radionuclide migration in the rock matrix [2, 3, 4]. Cs, which had been detected throughout all the core samples in this experiment, has been known to sorb selectively onto dark and mafic or altered minerals, i.e. biotite and chlorite [2, 4]. This study focused on possible effects of the microstructures such as micropores and mineral grains on the LTDE-SD results. Assuming a core sample, a 2-D model domain (24 mm × 93 mm) was formulated (Fig. 2). Due to lack of real data on the microstructures, their geometry was obtained from the polarizing micrograph on a thin section of gneiss sampled in the KAERI underground research tunnel. In order to avoid computational burden from simulating intergranular pore boundary with several μm of aperture, we incorporated the 1-D solute transport along them within the 2-D model domain. Inverse modeling in this work was carried out to find the five parameters of microstructures fitted to the LTDE-SD results: diffusion (D_e) and distribution coefficients (K_d) of the dark minerals located at fracture surface and rock matrix, respectively, and D_e of intergranular pore boundary.

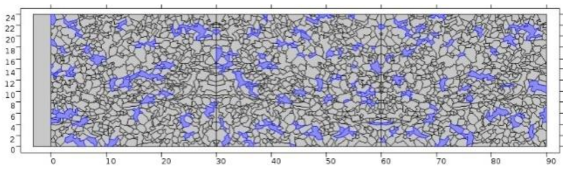

Fig. 2. 2-D Model domain with dark minerals (blue).

3. Results and Discussion

As shown in Fig. 3, both of the curves fitted with considering microstructures seems to be in accordance with the LTDE-SD results. The estimated parameters could be explained by the difference of Cs sorption on altered or unaltered minerals and the relatively fast diffusion along open mineral grain boundary. The fluctuation of penetration profile were highly relevant to the geometry of microstructures such as distribution and content of dark minerals and the connectivity of micropores. From this result, it is inferred that the high activity of steep slope in penetration profile of Cs resulted from its strong sorption onto the dark minerals located at the core surface directly exposed to the tracer cocktail. Also, due to the fast diffusion along the well-connected micropores, the tracer could reach the dark minerals located at the inner part of core sample and it might finally lead to the long tailing in the penetration profile.

4. Conclusion

This study provided a possibility that the microstructures in rocks leaded to the anomalous behavior of a tracer shown in the LTDE-SD results. One of the most influential factors on the simulation results must be the heterogeneity in geometry of microstructures. Particularly, it was observed on this work that the shapes of resulting curves were totally dependent on their geometry considered. This fact again highlighted that the microstructures could be critical to the fate of radionuclides in the rock matrix, as well as the LTDE-SD results. From this conclusion, additional modelling work on the effects of distribution and contents of mineral grains and connectivity of micropore networks is in progress.

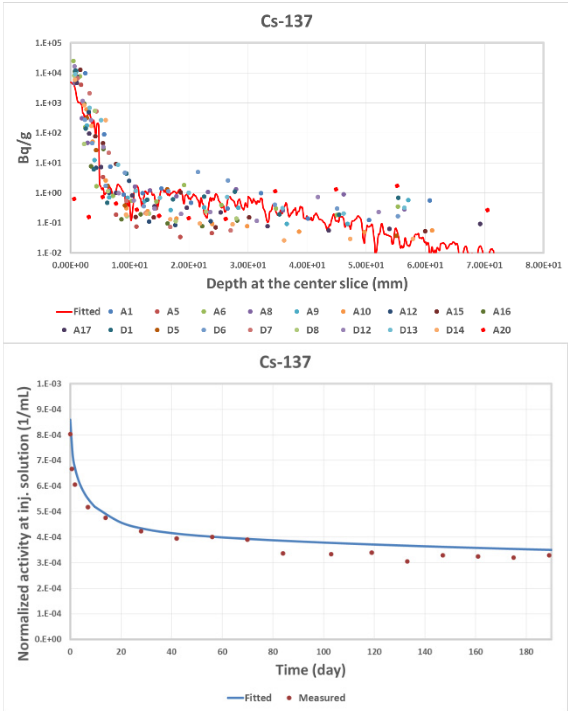

Fig. 3. Fitted results for penetration profile (upper) and temporal change in activity of tracer cocktail (lower).

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