Multi-species Diffusion Analysis in Na-beidellite under Various Dry Density and Temperature Conditions

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1. Introduction

Understanding the characteristics of long term transport behavior in porous media is essential in the assessment of radionuclide release through the backfill of high level radioactive waste (HLW) disposal facility. By calculating the movement of dissolved radionuclides through the backfill material or host rock, we can evaluate the impact and safety of the HLW facility for environment. Bentonite is a key component of the engineered barrier system (EBS) of the facility, and diffusion is the most important transport mechanisms of radioactive species. We have introduced a new numerical analysis method using a molecular dynamics simulation (MD), a multiscale homogenization analysis (HA) for the diffusion process of some chemical species in bentonite. Microscale properties such as diffusion coefficient of each ion have been calculated by using MD. Macroscale properties were determined by using the HA method, and a FEM was applied for analyzing the macroscale diffusion process. Under various temperature (293, 323 and 353K) and dry density (1.2, 1.6, 2.0Mg/m^3) of bentonite, diffusion behaviors of $^{36}Cl^-$ and $^{125}I^-$ and Na ions of NaCl-Na-beidellite and NaI-Na-beidellite model were calculated. We compared the results with in situ and laboratory experimental data.

2. Procedure of Numerical Analysis

Diffusion properties of Na^+, I^- and Cl^- ions existing in NaCl-Na-beidellite/NaI-Na-beidellite water systems were calculated by MD simulations. Figure 1 shows obtained diffusion coefficients in the interlayer water of the beidellite/water system.

Macroscale diffusion coefficients have been calculated by using the MD/HA method under various dry density and temperature conditions. Finally, an FEM analysis for the multi-species diffusion problem was applied for the diffusion problem in bentonite by using the homogenized diffusion coefficients obtained by the MD/HA method.

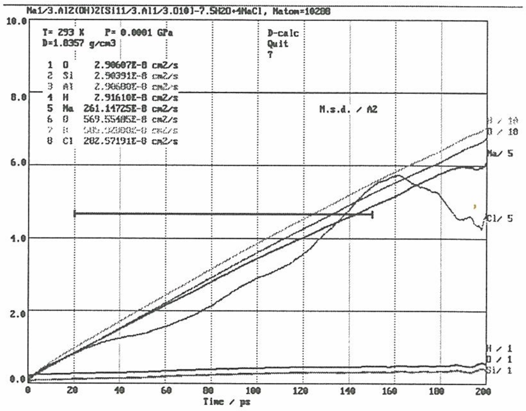

Fig. 1 Diffusion coefficients calculated by MD simulations

3. Results of Numerical Analysis

Dependence of Dry Density

Based on the MD/HA calculations we understand that the diffusion coefficient of each ion is inversely proportional to the dry density. Breakthrough curves of concentration, C_t/C_0, (C_t is the tracer concentration at time t and C_0 is the initial concentration in the reservoir) calculated by the FEM diffusion analysis using macroscale diffusion coefficients obtained by the MD/HA procedure are given in Figure 2 together with other experimental data ([2], [3], [4]). Figure 2 shows that both I^- and Cl^- diffuse slower as increasing the dry density and numerical results are well fitted with the experimental results.

Dependence of Temperature

Breakthrough curves of concentration due to temperature change are shown in Figure 3. We understand that the concentration profiles of I^- and Cl^- are proportional to the temperature at the same elapsed time.

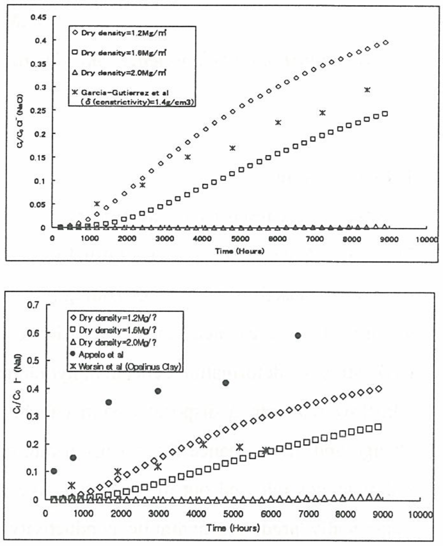

Fig. 2 C_t/C_0 results given by FEM (under

4. Conclusion

In this research, we introduced a new FEM analysis method using MD/HA results under various dry density and temperature conditions. That is, by the MD/HA procedure we calculated homogenized diffusion coefficients, and by introducing these results into a macroscale FEM analysis, the multi-species diffusion problem was solved. The results show that the diffusion profiles are proportional to the temperature and inversely proportional to the dry density.

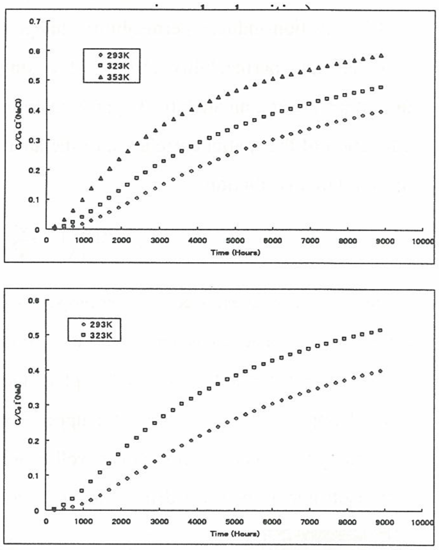

Fig. 3 C_t/C_0 results given by FEM (under various temperatures)

REFERENCES

[1] Mitchell, J.K., Soga, K., Fundamentals of soil behavior, *John Willy and Sons. Inc.*, (1992) 1-82.

[2] Appelo, C.A.J., Vinsot, A., Mettler, S., Wechner, S., Obtaining the pore water composition of a clay rock by modeling the in- and out-diffusion of anions and cations from in-situ experiment. *J. contaminant Hydrology*, (2008) 101:67-76.

[3] Wersin, P., Van Loon, L.R., Soler, J.M., Yiilera, A., Eikenberg, J., Gimmi, Th., Hermán, P., Boisson, J.-Y., Longterm diffusion experiment at Mont Terri: firsrt results from field and laboratory data. *Applied Clay Science*, (2004) 26:123-135.

[4] García-Gutiérrez, M., Cormenzana, J.L., Missana, T., Mingarro, M., Diffusion coefficients and accessible porosity for HTO and ^{36}Cl in compacted FEBEX bentonite. *Applied Clay Science*, (2004) 26:65-73.