Biogeochemical modelling of water-rock-microbe system in Horonobe area, Japan

T. IWATSUKI[1]*, Y. SASAKI[2], T. ITOH[2], T. ASANO[2], Y. AMANO[1], H. YOSHIKAWA[2], K. AOKI[1], T. NAKAMURA[3] AND T. NAGAOKA[3]

[1]Geological Isolation Research and Development Directorate, Japan Atomic Energy Agency, Horonobe, Hokkaido, Japan (*correspondence: iwatsuki.teruki@jaea.go.jp)
[2]Geological Isolation Research and Development Directorate, Japan Atomic Energy Agency, Tokai, Ibaraki, Japan
[3]Biotechnology sector, Central Research Institute of Electric Power Industry, 1646 Abiko, Chiba, 270-1194 Japan

Microbial activities and the reaction processes with groundwater and rock minerals up to 500 m below ground level were studied to infer the redox process and buffer capacity of rock materials for the articifitial disturbance such as facility construction at subsurface. Based on results of observation at *in situ* and batch experiments, the geochemical modelling using PHREEQC-2 was carried out to develop the numerical simulation techniques on water-rock-microbe interaction system.

The groudnwater in deep subsurface at Horonobe area is in reducing condition and the minerals such as carbonates, sulphides suggesting reducing condition omnipresents in rock matorix. Dominant microbes at the area are nitrogen-related bacteria, methanotrophs, and methanogens.

Batch (jar-fermentor) experiment using groundwater and rock minerals indicated that the redox potential changed from approx. +300 to -400mV after 8.5 days incubation in biotic condition, while the redox potential was in oxidizing condition with approx. +300mV for 40 days incubation in abiotic condition. Then the microbial activity would have an important role for the recovery of the reducing condition during the facility construction at subsurface.

In the theoretical calculation to reproduce the experimental results, the following hypothesis was made based on above results; the dominant microbial group changed in accordance with the redox condition; the dominant microbial groups were aerobes, iron reducers and fermenters. Thus the simulation results on the evolution of redox potential suggests that the PHREEQC-2 can be applied to describe the water-rock-microbe interaction system.

This study was performed as a part of 'Project for Assessment Methodology Development of Chemical Effects on Geological Disposal System' funded by Ministry of Economy, Trade and Industry, Japan.

Solvated hydronium and hydroxide ions: An *ab initio* dynamics view

SRINIVASAN S. IYENGAR

Department of Chemistry, Indiana University, 800 E. Kirkwood Ave, Bloomington, Indiana 47405, USA. iyengar@indiana.edu

The structure, dynamics, and spectroscopy of protonated, unprotonated, and hydroxide water clusters have remained an important challenge with fundamental implications in a variety of areas including environmental and biological sciences. In this contribution new computational results will be presented for a variety of protonated and hydroxide water clusters. These results are based on ab initio molecular dynamics which combines the dynamical evolution of nuclei with simultaneous computation of electronic structure. The structure, spectroscopy and surface propensity of these ions will remain the focus of this discussion with spectific attention to finite temperature and dynamical effects.