Geophysical Research Abstracts,
Vol. 11, EGU2009-1815, 2009
EGU General Assembly 2009

Reaction and Diffusion of Cementitious Water in Bentonite: Results of 'Blind' Modelling

C Watson (1), K Hane (2), D Savage (1), S Benbow (1), J Cuevas (3), and R Fernandez (4)

(1) Quintessa Ltd, The Hub, 14 Station Road, Henley-on-Thames, RG9 1AY, UK (firstnamesecondname@quintessa.org), (2) Civil Engineering Design Division, Kajima Corporation, 5-30 Akasaka 6-chome, Minato-ku, Tokyo 107-8502, Japan (hane@kajima.com), (3) Dept de Geologia y Geoquimica, Facultad de Ciencias, Universidad Autonoma de Madrid, Campus Cantoblanco, 28049 Madrid, Spain (jaime.cuevas@uam.es), (4) Instituto Eduardo Torroja, CSIC, C/Serrano Galvache, 4, 28033, Madrid, Spain (raul.fernandez@ietcc.csic.es)

The potential deleterious geochemical interactions of clay with cement/concrete may provide a constraint on the use of the latter material in deep geological disposal facilities for radioactive wastes. Consequently, it is important to have a fundamental understanding of these interactions to be able to assess their likely impact over the long timescales appropriate to the isolation of radioactive wastes from the human environment. Here, a laboratory experiment investigating the effects of cementitious water diffusing through bentonite has been simulated using a coupled reactive-transport geochemical modelling code. The modelling study was carried out before the results of the experiments were available, as an exercise in 'blind' modelling. A sensitivity study was carried out to investigate uncertainties associated with a number of input parameters, such as the precise nature of kinetic and ion-exchange reactions, diffusion coefficients, pore water composition, and montmorillonite dissolution models. The experiments used two types of fluid; one saturated with calcium hydroxide showed little mineralogical alteration, which was predicted by the computer simulations. A high pH K-Na-OH-based water however, caused alteration (pore blocking by hydrotalcite, gibbsite and brucite growth) to a depth of 2 mm in the bentonite after a period of 1 year. Experimental evidence showed that ion exchange of Mg-montmorillonite to K-montmorillonite was not confined to this thin region however, and was found to extend throughout the whole of the bentonite sample. The pore blocking by mineral precipitation and movement of ion exchange fronts through the bentonite were accurately simulated by the model.

The choice of dissolution model for montmorillonite played an important role in the outcome of the simulations. Of the cases considered in the sensitivity study, that employing the so-called 'Yamaguchi model' was clearly the best match, exhibiting all the main characteristics of the experiment, including pore blocking, brucite precipitation, minor montmorillonite dissolution, and the replacement of Mg- by K-montmorillonite throughout the length of the bentonite. Other factors (mineral growth rates, the smectite surface area, and the inclusion of trace minerals in the bentonite mineralogy) had a smaller impact upon the simulation results over the timescales considered. However, extrapolation of the results of the experiments and modelling to the timescales of interest for the isolation of radioactive wastes will require more realistic modelling of secondary mineral growth rates in the bentonite alteration process.