Geochemical modeling for boron removal by a permeable reactive barrier using magnesium oxide

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Geochemical models for boron removal by magnesium oxide was constructed from experimental results obtained in batch test [1]. Partial dissolution of magnesium oxide, precipitation of brucite and $MgB(OH)_5$, and complex ion formation of $MgB(OH)_4^+$ were considered. First order kinetics were also considerd for precipitation or disolution of these minerals. These models successfully expressed experimental results of pH and concentration of boron/magnesium ion in solution.
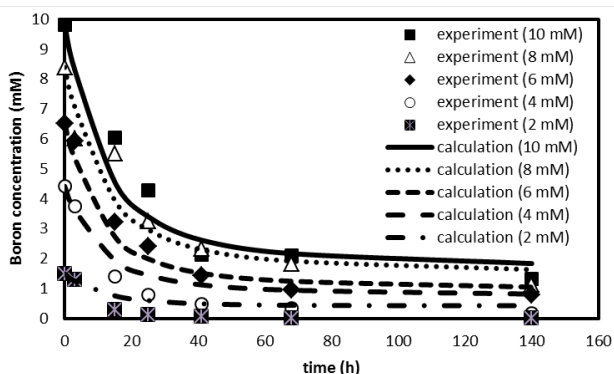
Figure 1: Comparison between experimental data and geochemical model analysis for boron concentarion change over time.

The above model was also confirmed to fit to the observed data in continuous column tests in combination with one dimensional advection-diffusion equation. This model is practically useful to predict the long term performance of PRB to treat borate using MgO for several decades.

[1] Sasaki *et al*. (2011) *J. Hazard. Mater* **185**, 1440–1447.

Physicochemical controls on adsorbed water film thicknesses in unsaturated porous media

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Large volumes of Earth's subsurface contain pores with water present as wetting films residing between mineral surfaces and a nonwetting fluid. These variably water-saturated environments include soils, deep unsaturated rock formations, and deep reservoirs containing hydrocarbons and CO_2. Water in these environments is retained by both capillarity and adsorption, with the adsorptive component most sensitive to solution chemistry and interfacial properties at both solid-water and water-fluid (gas, immiscible liquid, or supercritical fluid) interfaces. It is important to understand how the thickness of adsorbed water films varies with system properties because film thickness can control flow and transport within the aqueous phase, and because reactions at mineral surfaces are strongly influenced by the contacting fluid phase. The thickness of films is dependent on the component of the wetting phase chemical potential denoted the matric potential in soils and the disjoining (capillary) potential in deep reservoirs. The Derjaguin-Landau-Verwey-Overbeek (DLVO) theory combines electrostatic and van der Waals contributions to predict water film potential versus thickness relations, and is frequently applied in studies of mineral-water-mineral and mineral-water-hydrocarbon systems. However, adsorbed water films confined between mineral surfaces and nonwetting fluid phases are not present over the full range of disjoining potentials because a pore scale dependent threshold capillary pressure needs to be exceeded to allow coexisitence of both fluid phases in pores. In this study, capillary scaling [1] is used to predict ranges of matric (disjoining) potentials within which adsorbed water films can exist in gas-water-mineral systems and in supercritical CO_2-water-mineral systems [2]. We then apply DLVO models to calculate adsorbed water film thicknesses in these systems [3]. These calculations predict that under many conditions found in the subsurface, thicknesses of adsorbed water films are less than 20 nm. Moreover, the calculations predict a very wide range of potentials over which thicknesses of adsorbed films are less than 2 nm.

[1] Miller & Miller (1956) *J. Appl. Phys.* **4**, 324–332.
[2] Tokunaga (2009) *Water Resour. Res.* **45**, W06415.
[3] Tokunaga (in review, *Water Resour. Res.*)