Reactive Transport Modelling In Active Clays Using COMSOL Multiphysics®

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Abstract

The study of the movement of solutes and their interaction with the solid phase of active clays is a problem of maximum interest in various geoenvironmental engineering applications, but especially in the deep geological disposal of spent nuclear fuel and other highly radioactive materials. The modelling of the physicochemical phenomena that determine the reactive transport of solutes is complex due to the high number of couplings between the various processes that take place within the soil. To carry out this demanding task, only COMSOL Multiphysics® has been used due to the high adaptability and the ease of implementation of new partial and ordinary differential equations. A model of clayey soil with two structural levels, with Donnan equilibrium between them and with a multicomponent diffusion that considers the complex phenomena of electrostatic interaction existing in the active clays, has been considered. For the studied geochemical system, a total of 10 mass balance equations and 4 ordinary differential equations have been used for the description of the dissolution-precipitation kinetics of the main minerals present in the system and a total of 13 algebraic equations to solve the chemical speciation problem. This work presents a synthetic case of application based on a one-dimensional multicomponent dispersive-advective-diffusive transport experiment through MX-80 compacted bentonite. This synthetic case was adapted from the benchmarking exercise defined in Alt-Epping et al (2015). MX-80 bentonite is composed primary of Na-montmorillonite and typically contain quartz, feldspars, gypsum, and calcite as accessory minerals. The geochemical system is composed of 42 species classified in 32 secondary species, which are the reaction products of the combination of 10 master species (H+, Ca+2, Mg+2, K+, Na+, Cl−, SiO2, Al+3, SO2−4, HCO3−). The main differences between the chemical composition of the initial porewater and the infiltration solution are a higher Ca+2 concentration, a lower salinity (Na+ and Cl−) and a lower SO2−4 concentration in the infiltration solution. The initial porewater of the bentonite was in equilibrium with gypsum and calcite. Flux-type boundary conditions are applied to the inflow and outflow boundaries. Besides, to verify the model developed in the COMSOL Multiphysics environment, the results were compared with PHREEQC, the reference software in geochemical modelling. Very satisfactory results were obtained. The superior quality of the advective transport modelling by COMSOL Multiphysics compared to PHREEQC has also been verified. Finally, computational efficiency is also better because the model developed uses a monolithic approach that greatly reduces the number of time steps required for simulation.

Acknowledgements
The authors acknowledge funding support from: (i) the Ministerio de Economía, Industria y Competitividad from Spanish Government and the European Union through the project [BIA2017 - 89287-R (AEI/FEDER, UE)] and (ii) the Ministerio de Ciencia, Innovación y Universidades from Spanish Government through the Postdoctoral Grant [IJC-2018 - 035212] awarded to Dr. López-Vizcaíno.

References
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Figures used in the abstract

Figure 1 : Figure 1. (a) Scheme of the experimental setup. (b) Temporal evolution of the total concentration of main master species evaluated in the outflow point. Solid line: Comsol Results and markers: Phreeqc results