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Multi-component reactive transport in a claystone: Insights from a ten-year alkaline in situ injection experiment

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In the 90's, early calculations based on mass balance assumptions only, led to the conclusion that 0.2-1 m3 of bentonite are needed to buffer the chemical perturbation created by 1 m3 of concrete. If true, this conclusion would have been problematic for the storage concepts that rely on the properties of unaltered clay materials, and this explains why so much effort has been put in reactive transport modeling studies of the long-term evolution of clay-concrete interfaces. This effort has been reviewed with a focus on large-scale simulations at the repository gallery scale [*1*]. None of the reviewed studies considered the presence of species dependent diffusion coefficients (multi-component diffusion or MCD) and the presence of a diffuse layer in clayey and cementious materials. The consideration of MCD and of the presence of a diffuse layer is indeed computationally expansive, and few reactive transport codes are capable of handling it. Moreover, the parametrization of such a model must rely on preliminary models of relevant dataset. In this framework, a ten year in situ experiment has been operated in the Meuse Haute Marne Underground Research Laboratory, in which a high pH solution (pH~13.2) interacted with the Callovo-Oxfordian claystone. The complex evolution of the chemical composition of the test interval was modeled using CrunchClay [*2, 3*] in a cylindrical geometry with full consideration of MCD and presence of a diffuse layer in the claystone porosity. The modeling results gave insightful indications on the multi components diffusion and minerals reactivity in such a system, making possible to parameterize future simulations of the long term evolution of clay/cement interfaces.

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