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Reactive transport modeling for assessing coupled hydrogeochemical processes at interfaces in deep geological repositories: from the laboratory to the real world

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Abstract. Deep geological repositories with a multi-barrier concept are foreseen by various countries for the disposal of high-level radioactive waste. Simulation tools for a close-to-reality description of repository evolution scenarios are required, especially to resolve the challenging task of comparing and assessing the long-term safety of different repository concepts in different host rocks within the German site-selection process. Chemical, thermal, and pressure gradients at the interfaces of the different barriers in a repository can lead to mineral dissolution and precipitation, generating non-linear responses in transport and mechanical properties of barrier materials and host rocks. Reactive transport modeling (RTM) can be applied to investigate these perturbations and processes across temporal and spatial scales to assess subsurface evolution. Nevertheless, implementing RTM at the continuum scale while accounting for pore-scale heterogeneities and geometry evolution remains a challenge. Pore-scale simulations offer the potential to capture the complex evolution of porous media over a broad range of Peclet and Damköhler numbers, and they can be utilized to improve the RTM by using upscaling methods (Prasianakis et al., 2020). In this context, we developed "lab-on-a-chip" experiments, combining time-lapse high-resolution optical microscopy and confocal Raman spectroscopy to test extended constitutive equations to classically employed Archie's law to improve the description of changes in transport properties (e.g., diffusivity) in evolving porous media in RTM. The 3D Raman tomography of the porous media combined with pore-scale modeling enabled the derivation of upscaled transport parameters. Our results highlight the importance of calibrating pore-scale models with quantitative experiments prior to simulations over a wide range of Peclet and Damköhler numbers, whose results can be further used for the derivation of upscaled modeling parameters. The derived and parameterized constitutive equations based on simple systems have been tested in reactive transport models as a sensitivity case study to evaluate uncertainties in the predictions of the evolution of real subsurface systems such as clay–cement interfaces in deep geological repositories.

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