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Numerical analysis of heterogeneous diffusion in complex materials exemplified by radionuclide migration in the sandy facies of the Opalinus Clay

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Radionuclide migration in clay rocks such as Opalinus Clay (OPA) is dominated by molecular diffusion, which strongly depends on the pore network geometries. In the sandy facies of OPA (SF-OPA), this pore network is critically modified due to variable sedimentary composition and diagenetic products. Accurate modeling and simulation of radionuclide migration in heterogeneous clay rocks play a key role in the safety assessment of deep geological repositories for nuclear waste.

Here, we first introduce a cross-scale analytical workflow used to obtain the diversity of pore network geometries in various subfacies of SF-OPA (i.e., clay laminae, sand laminae, and carbonate lenses) [1]. The resulting generalized pore network geometries are applied in digital rock models to calculate effective diffusivities, using a combined upscaling workflow [2]. The derived diffusivities of each subfacies component are then implemented into a core-scale model based on segmentation of computed tomography (μ-CT) data for modeling the heterogeneous diffusion patterns. These results are finally validated with Positron emission tomography (PET) measurements [1]. Next, we investigate the influence of sedimentary and diagenetic heterogeneity on heterogeneous diffusion in SF-OPA from lamina scale to drill core scale [3]. We discuss the spatial and temporal evolution of heterogeneous diffusion and the influence of material heterogeneity, thus improving the understanding of heterogeneous diffusion in the SF-OPA at the core scale. Finally, we present a comprehensive analysis of representative elementary volume (REV), which is decisive for a meaningful continuum-scale simulation of radionuclide migration in heterogeneous clay rocks like SF-OPA [4]. We develop a method to correlate the 3D REV for diffusivity to the 2D representative elementary area for porosity. The applicability of our approach for clay rocks is validated by experimental data on the diffusion of tritiated water in the heterogeneous sandy facies of OPA. Overall, the generalizable approach presented here contributes to significantly improve the predictability of radionuclide migration in potential host rocks.

[1] Bollermann et al. (2022) *Chem. Geol.* 606, 120997.

[2] Yuan and Fischer (2021) *Tansp. Porous Media.* 138 (2), 245-264.

[3] Yuan and Fischer (2022) *Appl. Geochem.* 146. 105478.

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