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The influence of sedimentary heterogeneity on the diffusion of radionuclides in the sandy facies of Opalinus Clay at the geological scale

Chaofan Chen[1], Tao Yuan[2], Renchao Lu[1], Cornelius Fischer[2], Vanessa Montoya[1], Olaf Kolditz[1,3], and Haibing Shao[1]

[1]Helmholtz Centre for Environmental Research-UFZ, Permoserstr. 15, Leipzig 04318, Germany
[2]Department of Reactive Transport, Institute of Resource Ecology, Helmholtz-Zentrum Dresden-Rossendorf, 04318 Leipzig, Germany
[3]Applied Environmental Systems Analysis, Dresden University of Technology, Dresden 01069, Germany

Radionuclide migration in clay-rich formations is dominated by molecular diffusion due to the low permeability of the claystone. Accurate estimation of radionuclide migration in host rock using numerical tools plays a key role in the safety assessment of disposal concepts for nuclear waste. In the sandy facies of the Opalinus Clay (SF-OPA), the spatial variabilities of the pore network and compositional heterogeneities at the pore scale (nm to µm) cause heterogeneous diffusion at the core scale (cm to dm). Such heterogeneous diffusion patterns affect the migration of radionuclides in the various sedimentary layers even above the core scale (~m). Small-scale heterogeneities of diffusive transport could play an important role in upscaling to larger length scales of SF-OPA, particularly because of differences in sedimentary and diagenetic facies. Therefore, a meaningful estimation of radionuclide migration in the host rock above the core scale requires a comprehensive study of the influence of sedimentary layers on the heterogeneous diffusion.

In this work, we study the heterogeneous diffusion of radionuclides based on a two-dimensional (2D) structural model from the geological data of SF-OPA in the Mont Terri rock laboratory at the m-scale. As key parameters for the diffusive transport calculation, the effective diffusion coefficients in different sedimentary layers are quantified based on the developed upscaling workflow from pore- to core-scale simulation combined with the multi-scale digital rock models [1]. The heterogeneous effective diffusivities are then implemented into the large-scale structural model for diffusive transport simulation using the FEM-based OpenGeoSys-6 simulator. Results show that the various heterogeneous effective diffusivities under different mesh resolution (length scales) in the large-scale simulations strongly affect the evolution of radionuclides concentration in SF-OPA, especially in the vicinity of the canister. The sensitivity analysis focuses on the effects of length, bedding angle and thickness of the sedimentary layer on the spatio-temporal evolution of radionuclide concentrations. The numerical results provide insight into the heterogeneous diffusion of radionuclides, contributing to enhanced long-term predictability of radionuclide migration in the host rock of the deep geological repository.

[1] Yuan, Tao, and Cornelius Fischer. "Effective Diffusivity Prediction of Radionuclides in Clay Formations Using an Integrated Upscaling Workflow." *Transport in Porous Media* 138.2 (2021): 245-264.