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Flow field analysis towards improved predictability of diffusive flux in host rocks for radioactive waste

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The predictive power of numerical approaches for the analysis of flow fields and, e.g., radionuclide migration, depends on the quality of the underlying pore network geometry. Validation of the obtained simulation results can only be performed with a limited number of methods. Positron emission tomography (PET) is a suitable technique that has been established in geomaterial sciences in recent years. The employment of appropriate radiotracers allows the analysis of advective transport and diffusive flux in a variety of complex porous materials.

In addition to the visualization of time-resolved transport patterns, the quantitative and statistical analysis of transport controlling parameters is currently in the focus of investigations using PET techniques. First, local transport properties can be extracted from single voxels or voxel layers of the flow tomograms. Second, the analysis of spatially correlated data sets, e.g. density data from micro-computed tomography (μCT) analyses, is the focus of interest. The purpose is to statistically compare the range of material heterogeneity with the range of transport heterogeneity and to derive generalizable conclusions.

Using low-permeability potential host rock types for underground radioactive waste repositories as examples, we analyzed the heterogeneity of the flow field at the laboratory scale [1]. Reliable predictions of diffusive flux heterogeneity are critical for assessing sealing capacity. We identified diagenetic and sedimentary subfacies components based on the concentration of diagenetic minerals and grain size variability, and quantified their pore size distributions and pore network geometries. The resulting generalized pore network geometries are used in digital rock models to calculate effective diffusivities, using a combined upscaling workflow for transport simulations [2]. Diffusion experiments analyzed with PET confirmed the simulation results and provided quantitative insights into the heterogeneity of diffusive flux. We introduced a statistical treatment of the PET and μCT tomographic datasets based on the spatial variability of both PET tracer concentrations and rock density. Targeting a generalized applicability, we present and discuss results on diffusive flux in different lithotypes. The focus of the comparison is on quantitative analysis of propagation heterogeneity and the correlation with data characterizing compositional homogeneity. Here we discuss possibilities of statistical evaluation of data from μCT analysis and their potential for correlation with PET analysis methods.

Participation

In-Person

References

[1] Bollermann, T.; Yuan, T.; Kulenkampff, J.; Stumpf, T.; Fischer, C., Pore network and solute flux pattern analysis towards improved predictability of diffusive transport in argillaceous host rocks. Chemical Geology 2022, 606, 120997.
[2] Yuan, T.; Fischer, C., The influence of sedimentary and diagenetic heterogeneity on the radionuclide diffusion in the sandy facies of the Opalinus Clay at the core scale. Applied Geochemistry 2022, 146, 105478.

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