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Unified computational workflow framework for radionuclide migration assessment in deep geological repositories in clay rock

Jaime Garibay-Rodriguez[1], Renchao Lu[1], Chaofan Chen[1], Haibing Shao[1], Olaf Kolditz[1,2,3], and Vanessa Montoya[1]

[1]Helmholtz-Zentrum für Umweltforschung GmbH - UFZ, Environmental Informatics, Leipzig, Germany (jaime.garibay-rodriguez@ufz.de)

[2]Technische Universität Dresden, Dresden, Germany

[3]TUBAF-UFZ Centre for Environmental Geosciences, Germany

In the context of deep nuclear waste disposal, a critical aspect in their safety assessment is the potential radionuclide release and migration into the geosphere during the required long period of disposal times. It is established that the multi-barrier system of underground repositories for nuclear waste will provide retardation for radionuclides migration. In this context, the understanding of the sorption mechanisms of radionuclides onto mineral surfaces (i.e., montmorillonite, illite) is essential [1]. On the other hand, reactive transport mechanistic-based radionuclide migration simulations, typically for 1 million years, pose a computational challenge. Surrogate-based simulations can be useful to enable sensitivity/uncertainty analysis that would be prohibitive otherwise from a computational point of view. Considering the current challenges in modelling radionuclide migration in low permeable clays and the importance of the results and implications of these simulations in socio-political decisions, it is necessary to provide appropriate computational tools in a transparent and easy-to-use way. In this work, we aim to provide such tools in a framework that combines the simulation capabilities of OpenGeoSys6 for radionuclide diffusion in porous media and the approachable nature of Project Jupyter [2] (i.e., JupyterLab), which provides a modular web-based environment for development, simulation and data integration. Several examples of the migration of different sorbing and non-sorbing radionuclides in a clay host rock for 1 million years are shown. Simulations results are obtained by using two numerical approaches, i) adopting a mechanistic model with multiple chemical species through OpenGeoSys-6#iPHREEQC and ii) the so-called single species approach by employing a pre-calculated look-up table to speed up the simulations [3]. In this way, we aim to promote the collaborative research of radionuclide migration assessment and, at the same time, to guarantee the availability and reproducibility of the scientific outcome through the OpenGeoSys initiative [4].

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