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A concept for integrating geological heterogeneity and ML surrogates into safety-assessment workflows

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The safe disposal of high-level radioactive waste requires robust far-field models treating crystalline rock as the ultimate containment barrier. Incorporating rock heterogeneities across scales makes radionuclide retention modeling more realistic but significantly increases computational demand, especially for 3D computations. To keep runtimes manageable while retaining physical fidelity, the MALEK project (Machine Learning for Complex Hydrological-Geochemical Processes in Crystalline Rock Repositories) aims to accelerate coupled thermal-hydro-mechanical-chemical (THMC) processes using machine-learning surrogates, ultimately supporting digital twin concepts for site selection.

In contrast to many ordinary ML applications, the main challenge for deep geological repositories is maintaining transparency regarding why certain results are obtained. This contribution presents challenges of transferring knowledge and workflows from manual processing chains to automated frameworks and trustable surrogate functions. Building on earlier work from the SANGUR and PREDIS projects as well as the EURAD programme, we use the example of calculating the distribution coefficient Kd from real rock samples. The calculation of Kd values for radionuclides in crystalline rock systems follows a multi-step workflow integrating geological, hydrogeochemical, and computational elements. For example, specific rock heterogeneities are simulated to obtain a comprehensive overview of possible mineral compositions. Then the aqueous phase is estimated and/or simulated before conducting chemical modelling through Geochemist's Workbench, drawing on established databases that provide thermodynamic and kinetic parameters for surface sorption and complexation reactions—most notably the RES3T data bank.

By presenting this workflow, the contribution highlights how important it is to maintaining the transparency required for safety assessment in deep geological repository projects in automated processing chains including surrogate models to deliver traceable and defensible Kd values. The concepts developed within the MALEK framework could thus contribute to the broader objective of building trustable digital twins that can support and accelerate the site selection process for radioactive waste repositories.