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# Modelling radionuclide transport in highly heterogeneous media and under variable hydrochemical conditions using a "dynamic Kd" approach

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Due to the high heterogeneity of fractured media and the ubiquitous lack of a complete site characterization, deterministic simulations of radionuclide transport in fractured rocks are notoriously highly uncertain. This uncertainty is usually addressed using stochastic methods; e.g. the connectivity structure of the medium is described using multiple realizations of Discrete Fracture Networks (DFN), which are then combined to particle tracking simulations. In these formulations, many complex geochemical retention processes are typically lumped into a single parameter: the distribution coefficient (Kd). This approach relies on an important assumption: the Kd values are constant in time. This hypothesis is critical under long-term geochemical changes as it is known that the distribution coefficient depends on the pH, redox conditions and major chemistry of the system. In this work, we present a novel methodology that combines the robustness of stochastic methods with an explicit description of water-solute-rock interaction processes. The reconciliation of all these is achieved by using a dynamic Kd approach. The hydrogeochemical evolution of the site of study is first computed using long-term and large-scale mechanistic reactive transport simulations. The simulated hydrochemical conditions are then used to generate a complete database of Kd values, which represent the hydrochemical conditions in every position and time of the model domain. Then, MARFA (Painter and Mancillas, 2009) is used to carry out Time Domain Random Walk (TDRW) simulations of radionuclide transport. In these simulations, Kd values are dynamically updated using the afore-mentioned database. The results (i.e. radionuclide breakthrough curves) bring the signature of the underlying changes in the background geochemistry.