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Quantification of crystal surface reactivity using positron emission tomography (PET) techniques

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Predicting the migration behavior of dissolved contaminants in the pore space of rock and soil is crucial for assessing the feasibility of remediation and long term waste storage strategies.

Positron emission tomography (PET) using conservative radiotracers is an established and reliable method for investigating advective flow and diffusive flux in porous geomaterials and for validating transport models [1, 2]. However, solute transport is often significantly influenced by sorption effects. Reliable data concerning these effects are crucial for analyzing remediation processes as well as predicting desired immobilization in waste storage applications.

To understand and quantify the effects of solute-mineral surface interactions, analyses beyond breakthrough curve measurements are essential. PET techniques offer unique capabilities by providing in-situ tracer propagation and concentration data with high temporal and spatial resolution, surpassing traditional flow and lysimeter experiments.

For many materials, it is desirable to quantify both reactivity and hydrodynamic flow. The simultaneous quantification of both effects requires the use of a dual tracer system. In this presentation, we discuss the possibilities of utilizing a tracer pair consisting of ^{18}F as a reactive tracer and ^{76}Br as its conservative counterpart. This allows the prediction of spatially resolved surface reactivities as well as the evaluation of advective flow. Using different sandy sediments as model systems, we demonstrate the quantifiability of localized sorption effects as low as 10 pmol/mm^3 .

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References

[1] J.L. Pingel, J. Kulenkampff, D. Jara-Heredia, M. Stoll, W. Zhou, C. Fischer, T. Schäfer, In-situ flow visualization with Geo-Positron-Emission-Tomography in a granite fracture from Soultz-sous-Forêts, France,

Geothermics 111 (2023) 102705. [2] T. Bollermann, T. Yuan, J. Kulenkampff, T. Stumpf, C. Fischer, Pore network and solute flux pattern analysis towards improved predictability of diffusive transport in argillaceous host rocks, Chemical Geology 606 (2022) 120997.

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