Modeling radionuclide sorption for crystalline rocks using real samples: Challenges and sources of uncertainty

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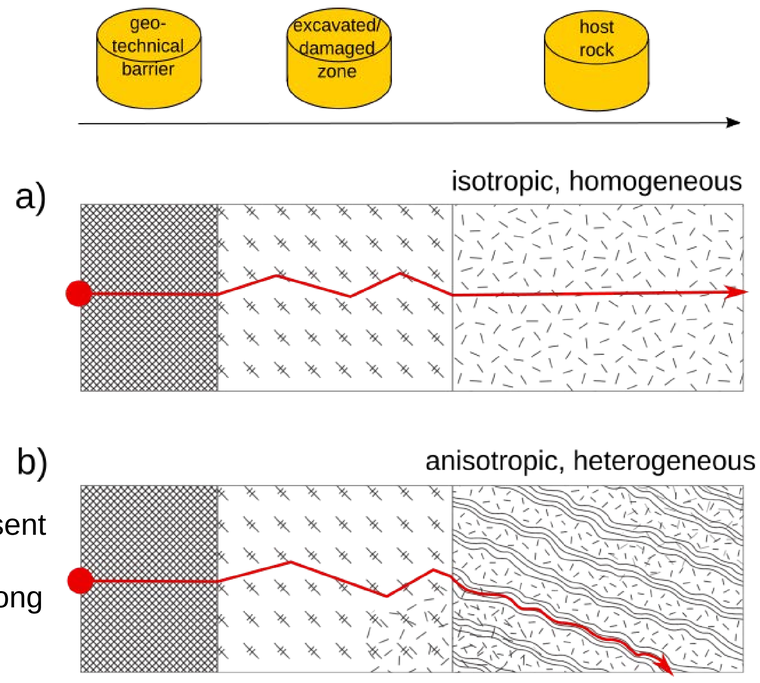
Motivation



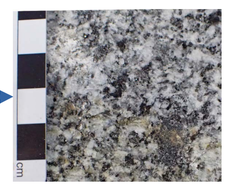
State of the art of far field model

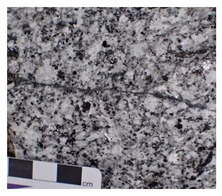
Our goal: present a model for mineralogy along pathways

Alterations of minerals

Variable grain sizes

Fracture filling along migration paths





Photos: A. D. Renno

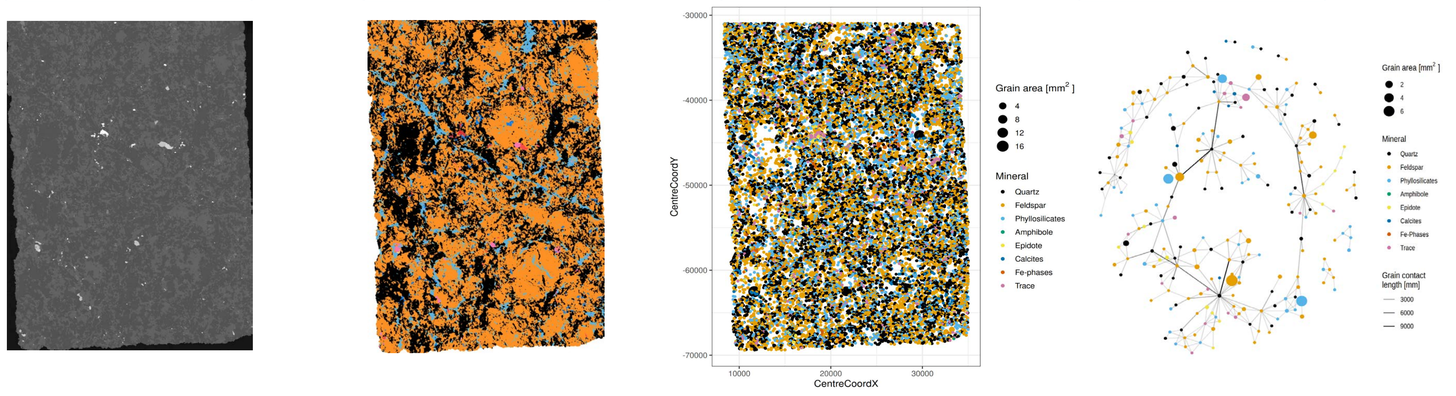
Safety of nuclear waste repositories depends on realistic predictions of radionuclide migration.

We aim to improve the estimation of radionuclide retention potentials of granitoid rocks

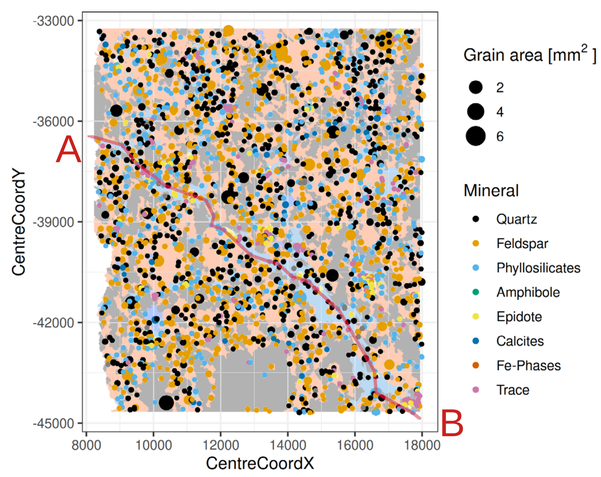
From rock sample to “effective” mineral surface

Measurement to graph …

BSE + EDS → Interpreted petrology → Geometric properties → Graph



… to mineral composition



- Measurement by Mineral Liberation Analysis (MLA): Back scattered electron (BSE) image in combination with Energy-dispersive X-ray spectroscopy (EDS)
- Information about mineral phases, voids, spatial distribution, grain sizes, grain contacts, etc. as data

- A rock containing *N* grains is given by an undirected graph $G = (V, E)$.
- Vertices $V = \{v_1, \ldots, v_N\}$ represent the grains.
- Edges $E = \{e_{i,j}\}$, $i, j = \{1, \ldots, N\}$, represent the contacts between the grains.

- Migration paths are described by a subgraph connecting the starting grain A and the ending grain B of the path.
- Results into modal mineralogy of the exposed surface along potential fluid migration path.

Calculation of distribution coefficients (K_d)

Workflow

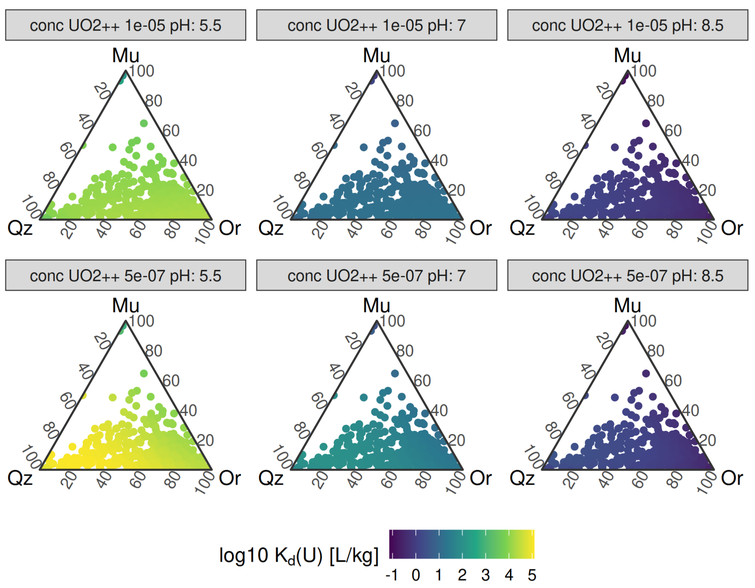
- “effective” mineral composition along migration path
- Fracture/pore network analysis: Volume of fluid in contact with rock mass
- Chemistry of aqueous phase/ fluids (element composition, pH, Eh, etc.)
- Surface complexation models for each mineral phase and element in fluid

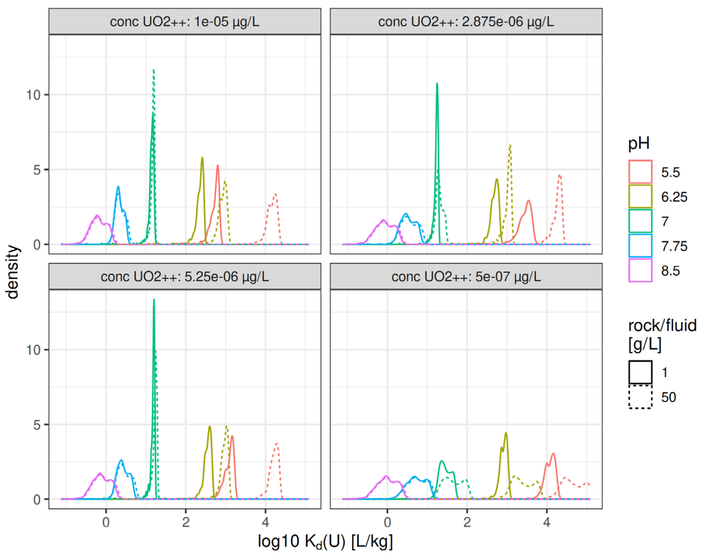
→ Geochemical modelling, e.g. by PhreeqC, GWB, etc.

RES³T Rossendorf Expert System for Surface and Sorption Thermodynamics

Results

Example for Qz – Mu – K-Fsp system -> **Distribution K_d values**





References

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RES³T-Rossendorf Expert System for Surface and Sorption Thermodynamics, Helmholtz-Zentrum Dresden-Rossendorf, www.hzdr.de/res3t

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