Modelling Platform for Multi-Field Processes in Deep Geological Repositories

Tage der Standortauswahl 2021, 11-12.02.2021

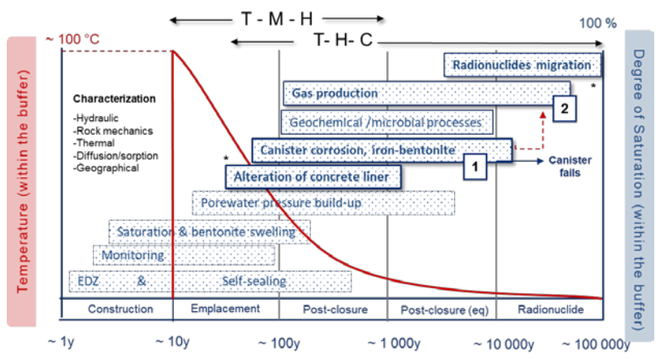
Coupled geochemical and multi-physical processes

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

[1]Department of Environmental Informatics, Helmholtz Zentrum für Umweltforschung - UFZ Leipzig GmbH, Germany,
[2]Faculty of Environmental Sciences, TU Dresden, Helmholtzstr., Dresden, Germany

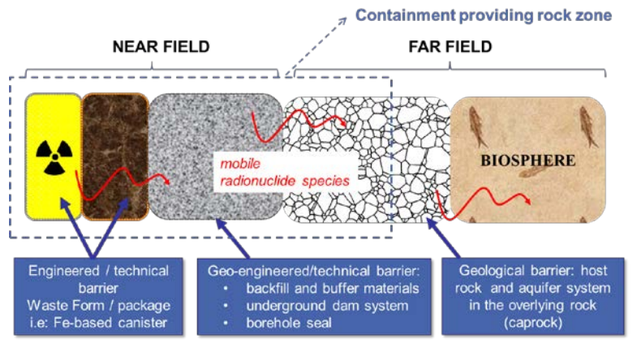
Temperature, saturation and coupled processes

Repository evolution vs time and space: Physical and Chemical processes taking place in the engineered barrier system will define the radionuclide mobility / retention.



Multibarrier system (materials)

Concrete, steel and clay are used as confinement barriers → During the prolonged period of disposal, they will undergo alterations



Coupling Scheme

$$\phi\frac{\partial c_i}{\partial t} + \nabla\cdot(\mathbf{q}c_i - \phi\mathbf{D}\nabla c_i) + Q_i + \boxed{R_i\left(c_1,...,c_n\right)} = 0.$$

Operator splitting approach

$$\int_\Omega N_k\phi N_j \,\mathrm{d}\Omega\,\frac{\partial\tilde{c}_i}{\partial t} + \int_{\Gamma_\mathrm{N}} N_k\bar{q}N_j\,\mathrm{d}\Gamma\tilde{c}_i - \int_\Omega \nabla^\mathrm{T}N_i\mathbf{q}N_j^\mathrm{T}\,\mathrm{d}\Omega\tilde{c}_i + \int_\Omega N_i\mathbf{q}\nabla N_j\,\mathrm{d}\Omega\,\tilde{c}_i - \int_{\Gamma_\mathrm{N}} N_k\phi\bar{J}_i\,\mathrm{d}\Gamma + \int_\Omega \nabla^\mathrm{T}N_i\phi\mathbf{D}\nabla^\mathrm{T}N_j\,\mathrm{d}\Omega\,\tilde{c}_i + \int_\Omega N_iQ_i\,\mathrm{d}\Omega = 0.$$

$$\int_\Omega N_k\phi N_j\,\mathrm{d}\Omega\,\frac{\partial\tilde{c}_i}{\partial t} + \int_\Omega N_kR_i\left(c_1,...,c_n\right)\,\mathrm{d}\Omega = 0.$$ ← Aqueous speciation, precipitation/dissolution, sorption, etc.

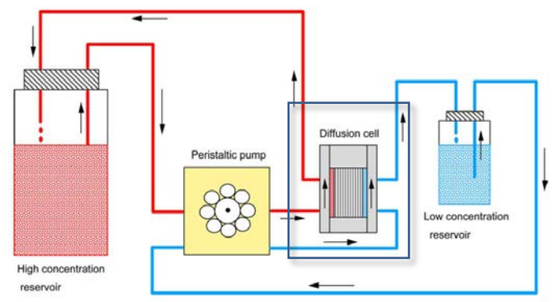
Benchmark: Cs^+ diffusion in Opalinus clay

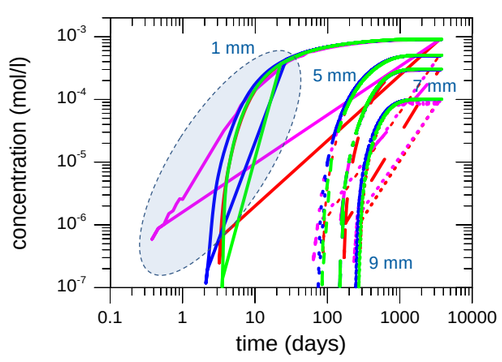
Can the migration of sorbing tracers in clayrock be predicted…?

Sorption equilibria
- 1- Mechanistic (multi species) or
- 2- Kd (single species)

+

Diffusion mass transport (compacted clay)





Benchmark of different numerical concepts: **25 times faster with the single species** concept than with the multi-species one

Better process understanding **of the geochemistry** and **deeper understanding** of the system to be analyzed.

Chemical evolution of engineered multibarrier systems

A numerical model to assess the hydro-chemical evolution of a **L-ILW disposal cell** in indurated clay rocks is developed.

Challenges: large spatial (2D) and temporal scales + highly complex chemical phenomena involving **cementitious materials.**

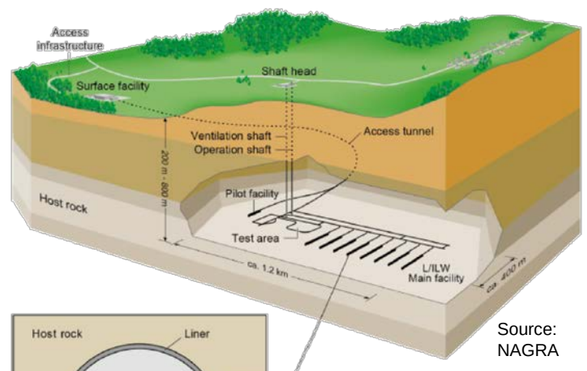
Source: ANDRA

Key outcome: the interaction of different components/materials and the expected hydraulic and/or **chemical gradients over 100 000 years** for disposal cell safety assessment.

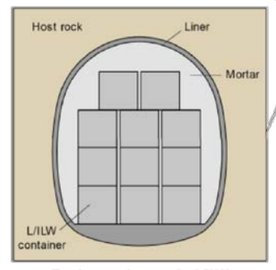
Methods: reactive transport modeling in `OpenGeoSys-6` coupled with `iPhreeqc`.

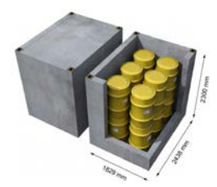
Transport + **Geochemistry**

- Transport → **Porosity-permeability** → **Diffusion**
- Geochemistry → **Aqueous and surface interactions** → **Solid phase evolution** → Impact on Diffusion

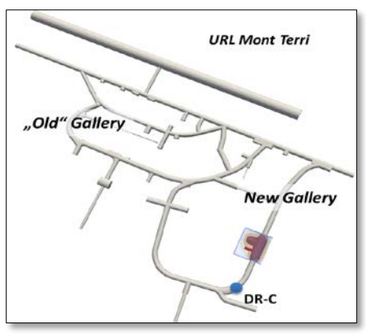


Source: NAGRA



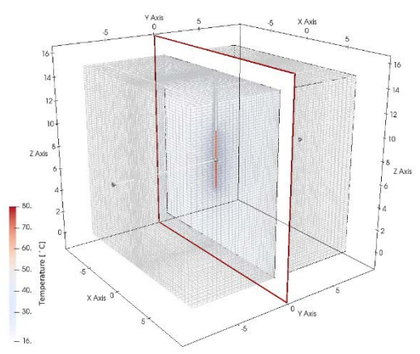


Radio-tracers diffusion in a thermal gradient in Opalinus Clay



→ **Mont Terri**

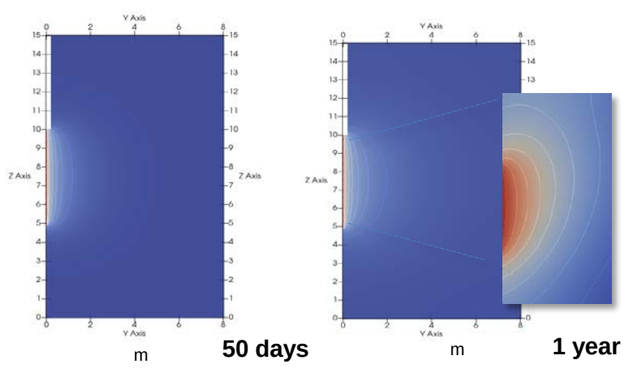
Tracers: HTO, ^{36}Cl, Br^-, $^{125}I^-$, $^{22}Na^+$, $^{137}Cs^+$, Cs^+, $^{85}Sr^{2+}$
→ very short half-life



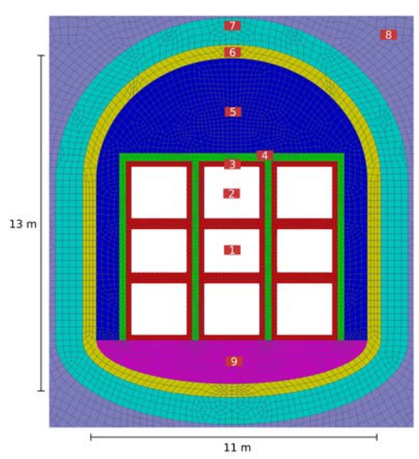
Conduction is the only heat transfer mechanism (intrinsic permeability ~ $1x10^{-19}$ m^2)

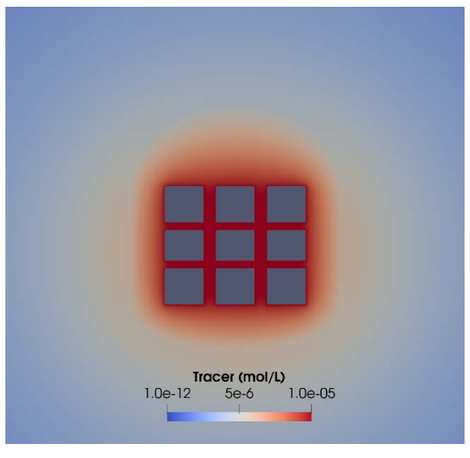
Anisotropy: 3D model

- Spacing between the boreholes **> 6 meters**.
- Over-coring of **400 mm** is possible after 1 year diffusion



Preliminary case: tracer diffusion in multibarrier system for 100 000 years.





Contact:
Dr. Vanessa Montoya
vanessa.montoya@ufz.de
Helmholtz-Centre for Environmental Research – UFZ Leipzig
Permoser Str. 15 04318 Leipzig

References:

[1] Lu et al. (2021). Water Resources Research (submitted)
[2) Aguila et al. (2021) Computational Geosciences (under review)
[3] Huang et al. (2021). npj Materials Degradation, 5, 4
[4] Idiart et al. (2020) Appl. Geochem. 115 , art. 104562

eurad European Joint Programme on Radioactive Waste Management
Bundesministerium für Bildung und Forschung
HELMHOLTZ RESEARCH FOR GRAND CHALLENGES