OpenGeoSys workflows

# The OpenGeoSys software framework for reactive transport and chemo-mechanical modeling in Deep Geological Disposal

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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.
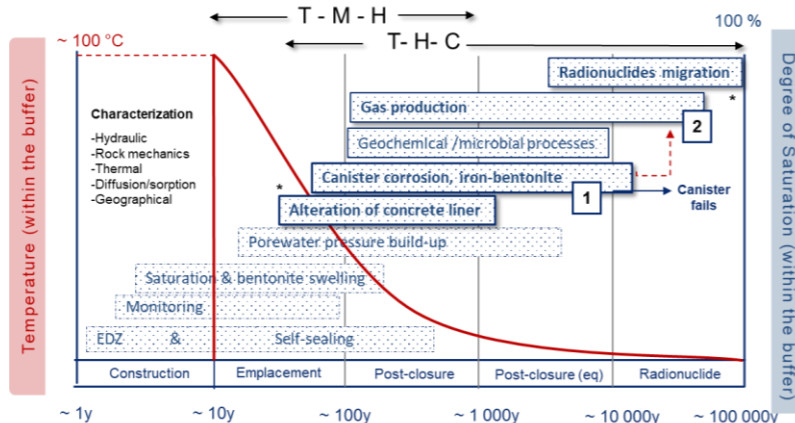
Multi-barrier system (materials)

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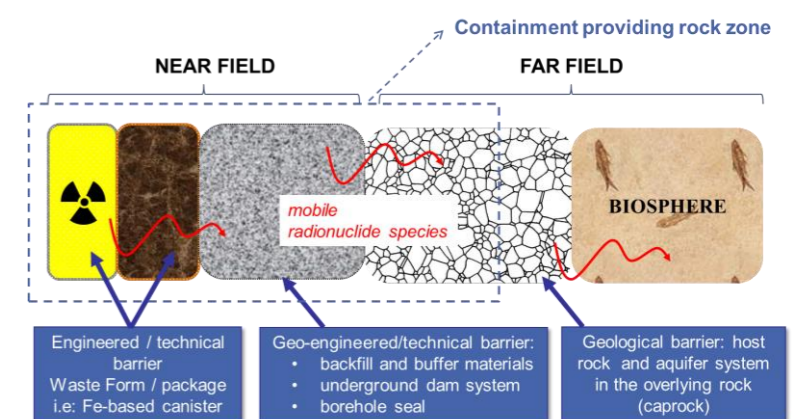
Coupling Scheme

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

Operator splitting approach

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

$$\int_\Omega N_k\phi N_j\,\mathrm{d}\Omega\,\frac{\partial \tilde{c}_i}{\partial t} + \int_\Omega N_kR_i\,(c_1, ..., c_n)\,\mathrm{d}\Omega = 0.$$ ← Aqueous speciation, precipitation/dissolution, sorption, etc
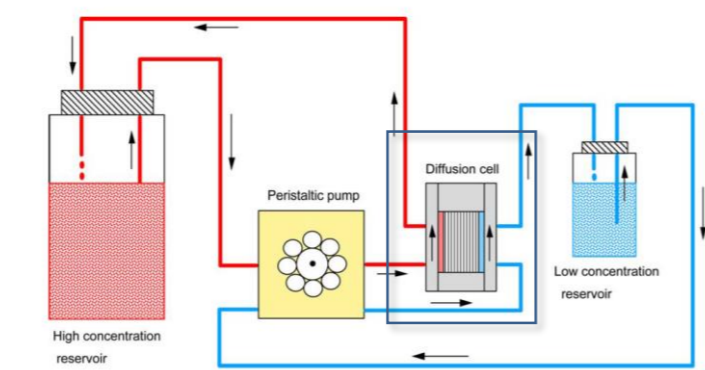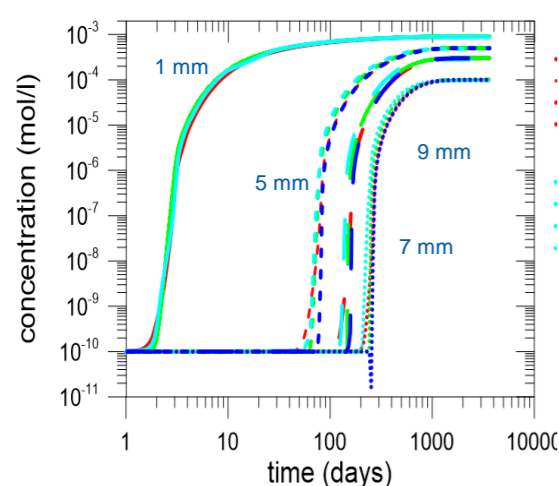
Benchmark: Cs+ diffusion in Opalinus clay

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.

— OGS — COMSOL — MCOTAC — CORE

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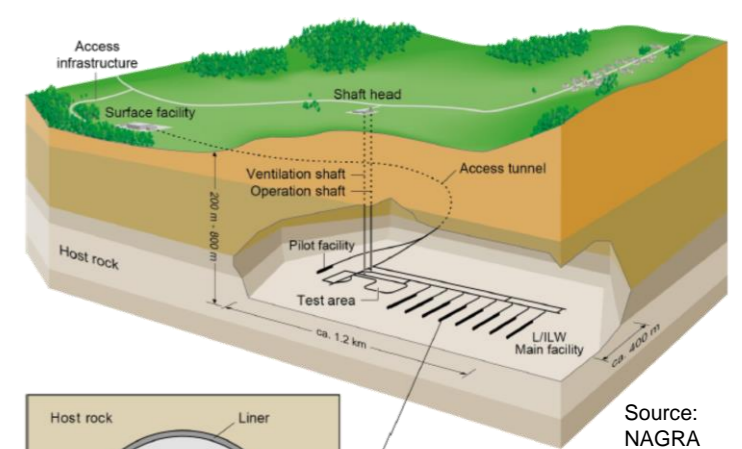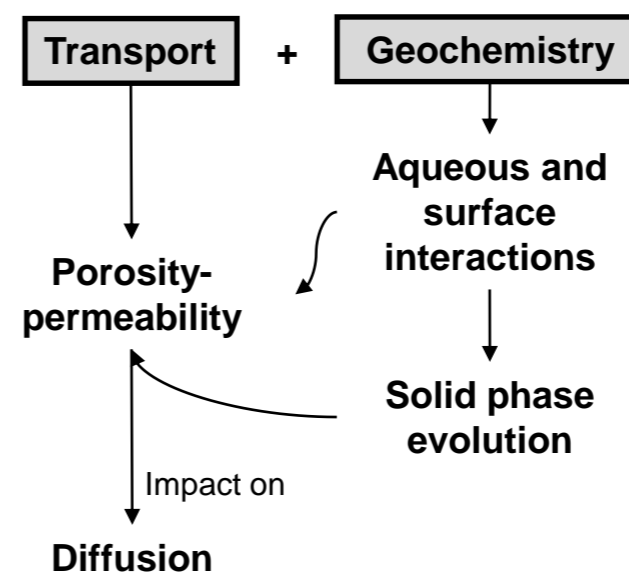
Challenges: large spatial (2D) and temporal scales + highly complex chemical phenomena involving **cementitious materials.**
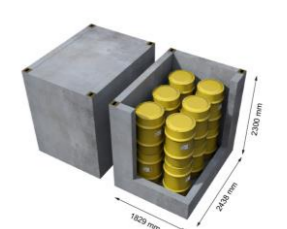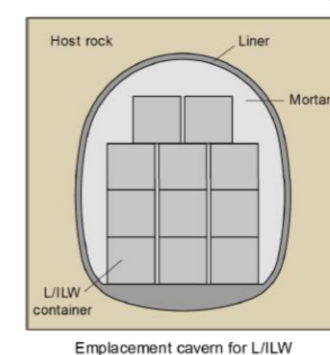

Source: ANDRA

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.
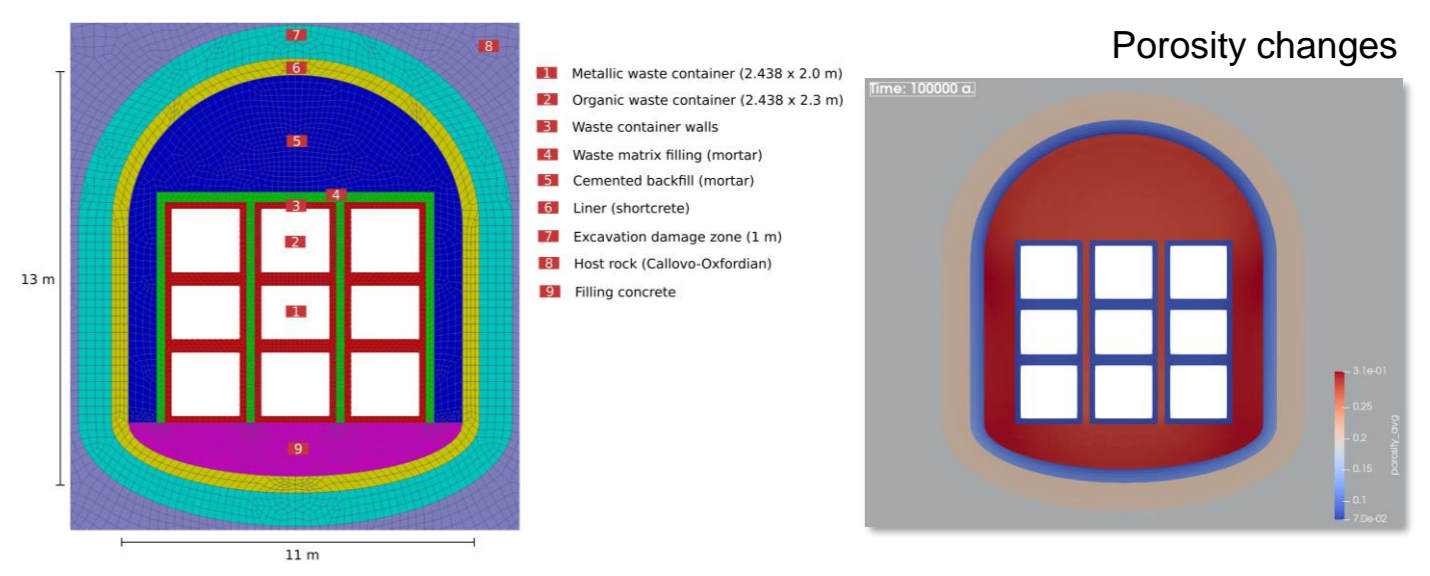
Methods: reactive transport modeling in OpenGeoSys-6 coupled with iPhreeqc.
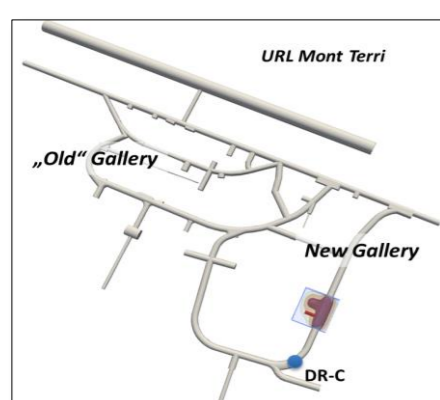
Transport + **Geochemistry**

Porosity-permeability

Aqueous and surface interactions

Solid phase evolution

Impact on

Diffusion

Source: NAGRA

Emplacement cavern for L/ILW

Reactive transport: Multibarrier system evolution for 100 000 years.

1. Metallic waste container (2.438 x 2.0 m)
2. Organic waste container (2.438 x 2.3 m)
3. Waste container walls
4. Waste matrix filling (mortar)
5. Cemented backfill (mortar)
6. Liner (shortcrete)
7. Excavation damage zone (1 m)
8. Host rock (Callovo-Oxfordian)
9. Filling concrete

Porosity changes
Time: 100000 a;

Radio-tracers diffusion in a thermal gradient in Opalinus Clay

URL Mont Terri
„Old" Gallery
New Gallery
DR-C

➔ **Mont Terri**

Tracers: HTO, ^{36}Cl, Br⁻, ^{125}I⁻, ^{22}Na⁺, ^{137}Cs⁺, Cs⁺, ^{85}Sr^{2+}
➔ very short half-life
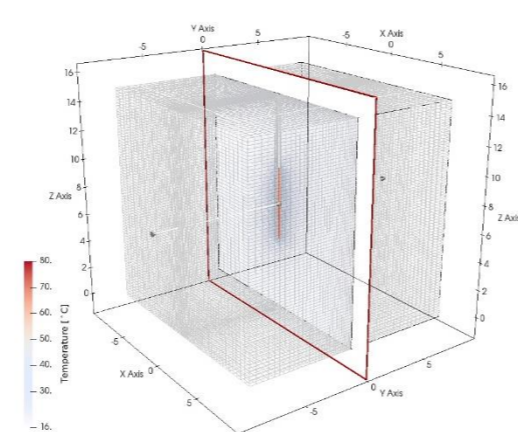
Conduction is the only heat transfer mechanism (intrinsic permeability ~ 1×10^{-19} m^2)

Anisotropy: 3D model

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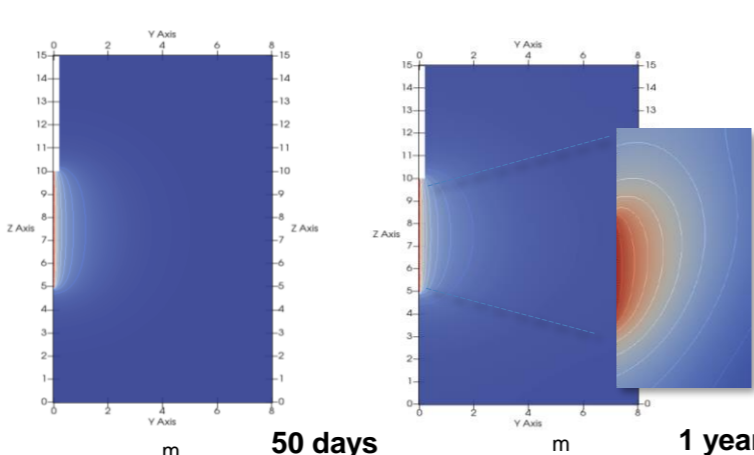
50 days   1 year

References:
[1] Lu et al. (2022). Computers & Geosciences 163, 105106
[2] Aguila et al. (2021) Computational Geosciences 25 (4), 1405-1436
[3] Montoya et al. (2021). EGU general assembly
[4] Garibay-Rodriguez (2022) Frontiers in Nuclear Engineering 1, 919541

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European Joint Programme on Radioactive Waste Management

Bundesministerium für Bildung und Forschung

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES