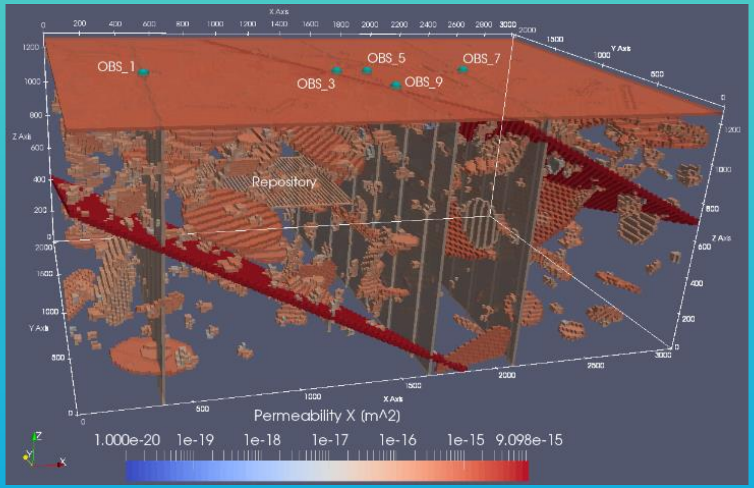
U.S. DEPARTMENT OF ENERGY | Office of NUCLEAR ENERGY

Spent Fuel and Waste Science and Technology (SFWST)

Clean. Reliable. Nuclear.




# Used Fuel Disposition in Crystalline Rocks

Nuclear Waste Technical Review Board fact finding Meeting 2020

Yifeng Wang
Distinguished Member of Technical Staff
Sandia National Laboratories

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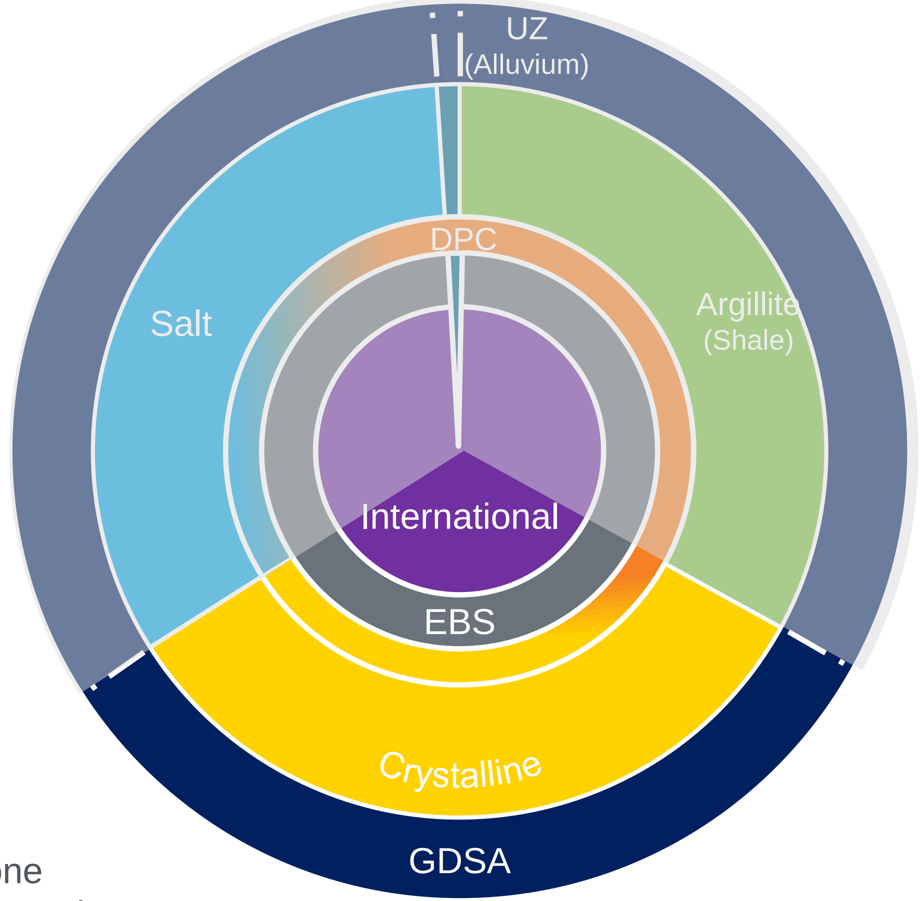
SAND2020-13111 PE

# Work package structure




UZ = Unsaturated Zone
DPC = Dual Purpose Canisters
EBS = Engineered Barrier System
GDSA = Geologic Disposal Safety Assessment

# Acknowledgments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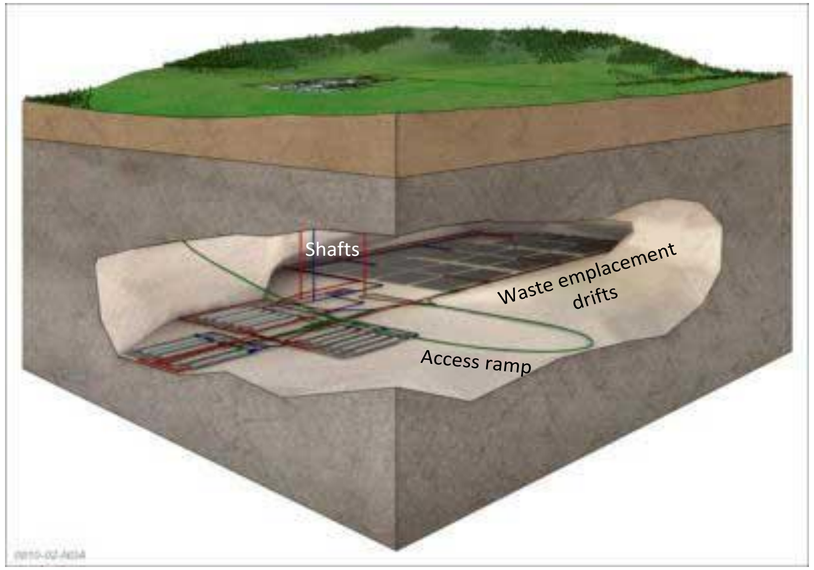
- H. Viswanathan, S. Chu, A. R. Hoinville, J. Hyman, S. Karra, N. Makedonska, K. Telfeyan, *Los Alamos National Laboratory (LANL)*
- Y. Guglielmi, C. Chang, P. Cook, P. Dobson, F. Soom, S. Nakagawa, C.-F, Tsang, S. Borglin, C. Doughty, L. Zheng, *Lawrence Berkeley National Laboratory (LBNL)*
- M. Zavarin, E. Balboni, C. Atkins-Duffin, W. Bourcier, S.F. Carle, K. Smith, C. Booth, *Lawrence Livermore National Laboratory (LLNL)*

# Characteristics of host rocks

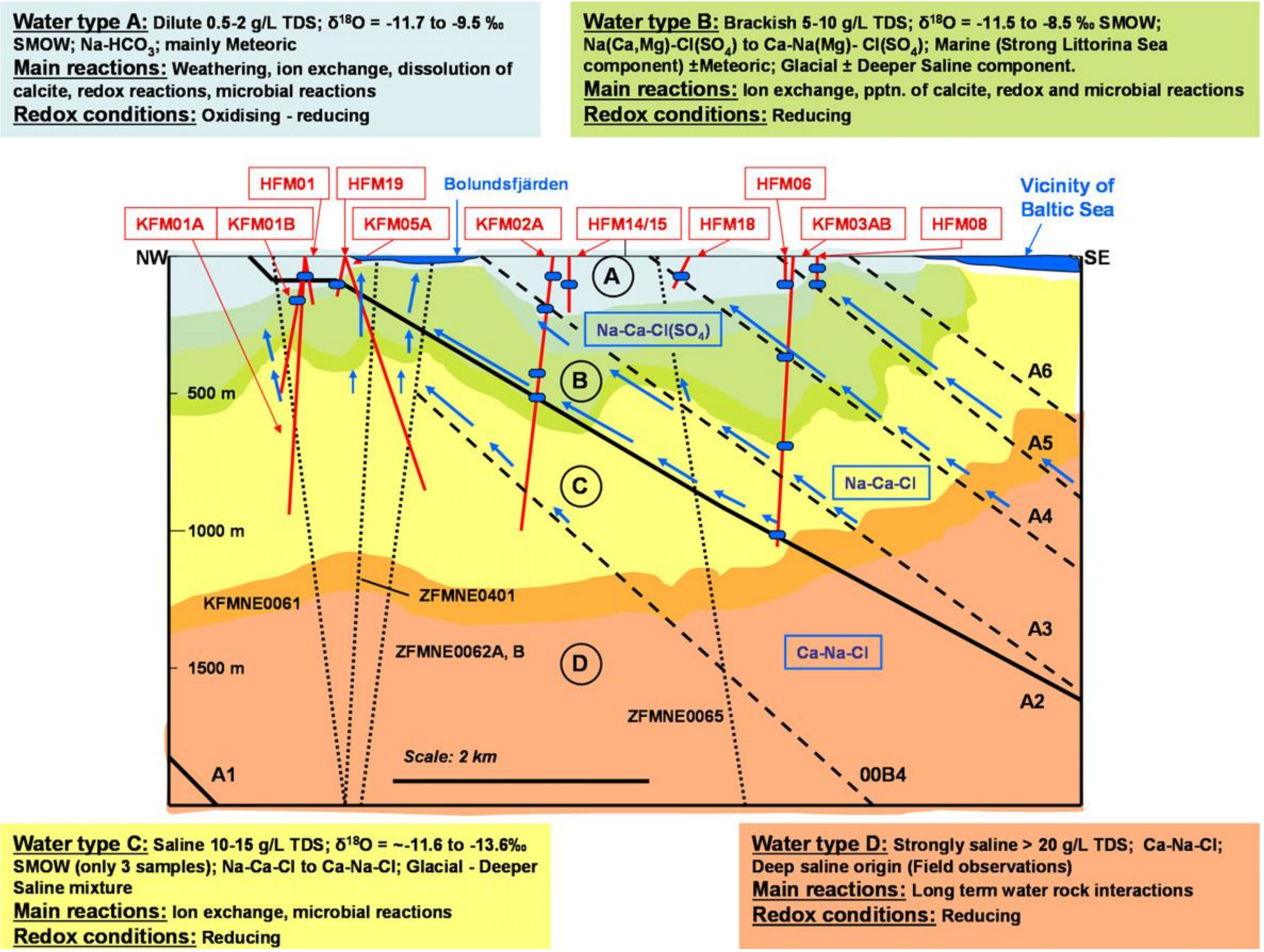
| Attributes | Salt | Shale | Granite (crystalline rock) | Deep boreholes |
|---|---|---|---|---|
| **Thermal conductivity** | High | Low | Medium | Medium |
| **Permeability** | Low | Low | Low (unfractured) to permeable (fractured) | Low |
| **Mechanical strength** | Low | Low | High | High |
| **Deformation behavior** | Visco-plastic | Plastic to brittle | Brittle | Brittle |
| **Stability of cavity** | Low | Low | High | Medium to high |
| **Dissolution behavior** | High | Very low | Very low | Very low |
| **Chemical condition** | Reducing; high ionic strength; relatively simple chemical system | Reducing; complex chemical system | Reducing; relatively simple chemical system | Reducing; relatively simple chemical system; moderate to high ionic strength |
| **Radionuclide retention** | Very low | High | Medium to high | Medium to high |
| **Thermal limit** | Relatively high | Relatively low (?) | No limit | No limit |
| **Available geology** | Wide | Wide | Wide | Wide |
| **Geologic stability** | High | High | High | High |
| **Engineered barrier system** | Minimal; waste package damage by room closure | Minimal; waste package damage by room closure | Needed. Able to fully take credit for the engineered barrier system | Borehole seal needed |
| **Human intrusion/resource exploration** | Relatively high | Relatively high | Low | Low |
| **Retrievability of waste** | Feasible | Feasible | Easily retrievable | Difficult |

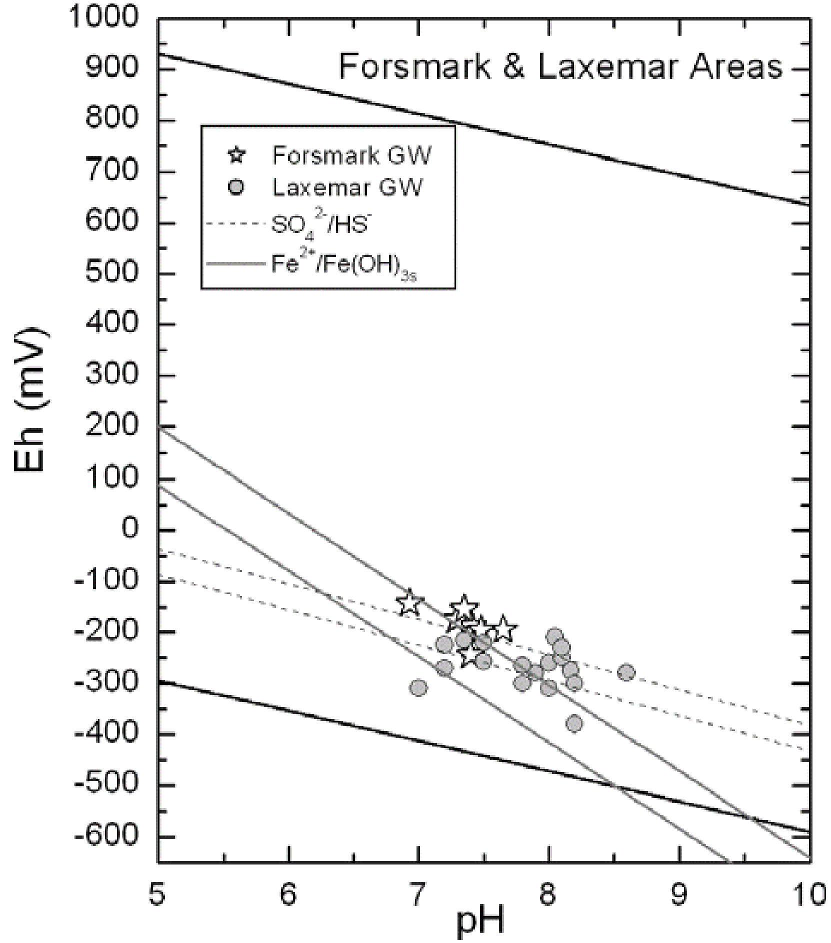



Modified from http://www.bbc.com/news/uk-england-cumbria-21253673

- High mechanical strength and thermal limit
  - Suitable for disposal of large and hot waste canisters
- Fractured nature
  - Engineered barrier system equally important as the nature barrier

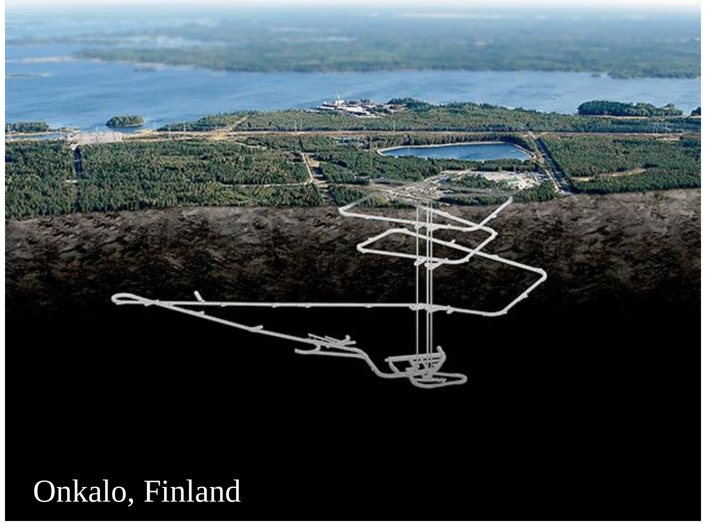
# Geochemical characteristics of groundwater




Laaksoharju et al. (2008)

# Disposal concept

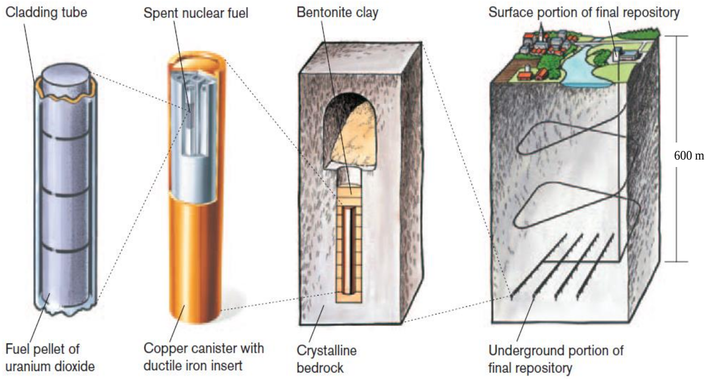

Onkalo, Finland

https://spectrum.ieee.org/energywise/energy/nuclear/nuclear-waste-deep-storage-plans-approved


Forsmark, Sweden

World-nuclear-news.org

https://www.wsj.com/articles/a-100-000-year-tomb-for-finlands-nuclear-waste-1485253831




Emplacement in tunnel boreholes (KBS-3 concept) (modified from SKB, 2011)

# Post-closure safety strategy

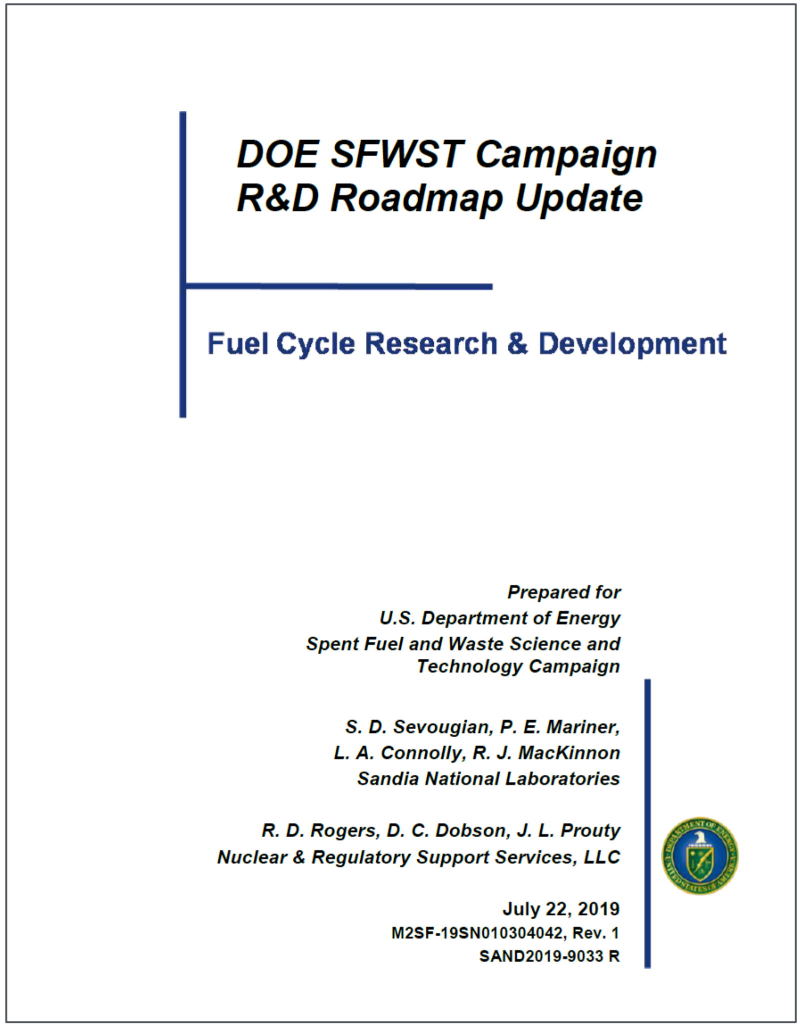
**Objectives:** Advance understanding of long-term disposal of used fuel in crystalline rocks (granitic or metamorphic rocks) and develop experimental and computational capabilities to evaluate various disposal concepts in such media.

- Assist the geologic disposal safety assessment (GDSA) team to develop a robust repository performance assessment model.
- Provide the GDSA with a basic “minimal” set of process models and model feeds to support the GDSA.
- Develop basis for process modeling that enables streamlined integration with system modeling resulting in feeds to GDSA.
- Consolidate model parameter data, especially thermodynamic data, to ensure more consistent usage of the data across the project.
- With the existence of different approaches taken by various researchers there is a need to understand how well the models are developed in terms of pedigree and rigor.
- Fully leverage international collaborations for data collection and model development and validation.
- Closely collaborate with other work packages, especially those on disposal in argillite and engineered barrier system design.

The current work focuses on: (1) better characterization and understanding of fractured media and fluid flow and transport in such media, and (2) designing effective engineered barrier systems (EBS) for waste isolation.

# Technical gaps and priorities mapped to R&D roadmap

- Fuel matrix degradation model (FMDM). Account for the effect of metal corrosion (jointed with argillite work package) (ANL). (H: D-05, E-14)
- Radionuclide interactions with corrosion products, especially Pu sorption and incorporation into magnetite and green rust (LLNL). (H: D-05, E-14)
- Bentonite erosion and colloid generation and their impact on radionuclide transport (LANL). (H: C-15, M-H: E-20)
- Fluid flow in low-permeability media (SNL, LBNL). (H: I-08, M-H: C-11)
- Long-term (up to months) temperature-controlled (up to ~200° C) flow and mechanical (and chemical) experiments on multiple core-scale samples; radionuclide interaction with bentonite (SNL, LBNL). (H: C-15, M: C-08)
- New-generation buffer materials/waste package materials; understanding thermal limits of buffer materials (SNL). (H: C-15, C-16, E-11, E-17)
- Discrete fracture network (DFN) model; especially a reduced order model for GDSA (LANL). (M-H: C-01, P-02)
- Workflow for field data synthesis and flow modeling in fractured media (SNL). (M-H: C-01, M-H: C-13, P-02)
- Geophysical and well-testing techniques for characterizing fractures and inflows; uncertainty reduction of key flow parameters in the EDZ (LBNL). (M-H: E-03)


**DOE SFWST Campaign R&D Roadmap Update**

**Fuel Cycle Research & Development**

*Prepared for*
*U.S. Department of Energy*
*Spent Fuel and Waste Science and Technology Campaign*

*S. D. Sevougian, P. E. Mariner, L. A. Connolly, R. J. MacKinnon*
*Sandia National Laboratories*

*R. D. Rogers, D. C. Dobson, J. L. Prouty*
*Nuclear & Regulatory Support Services, LLC*

July 22, 2019
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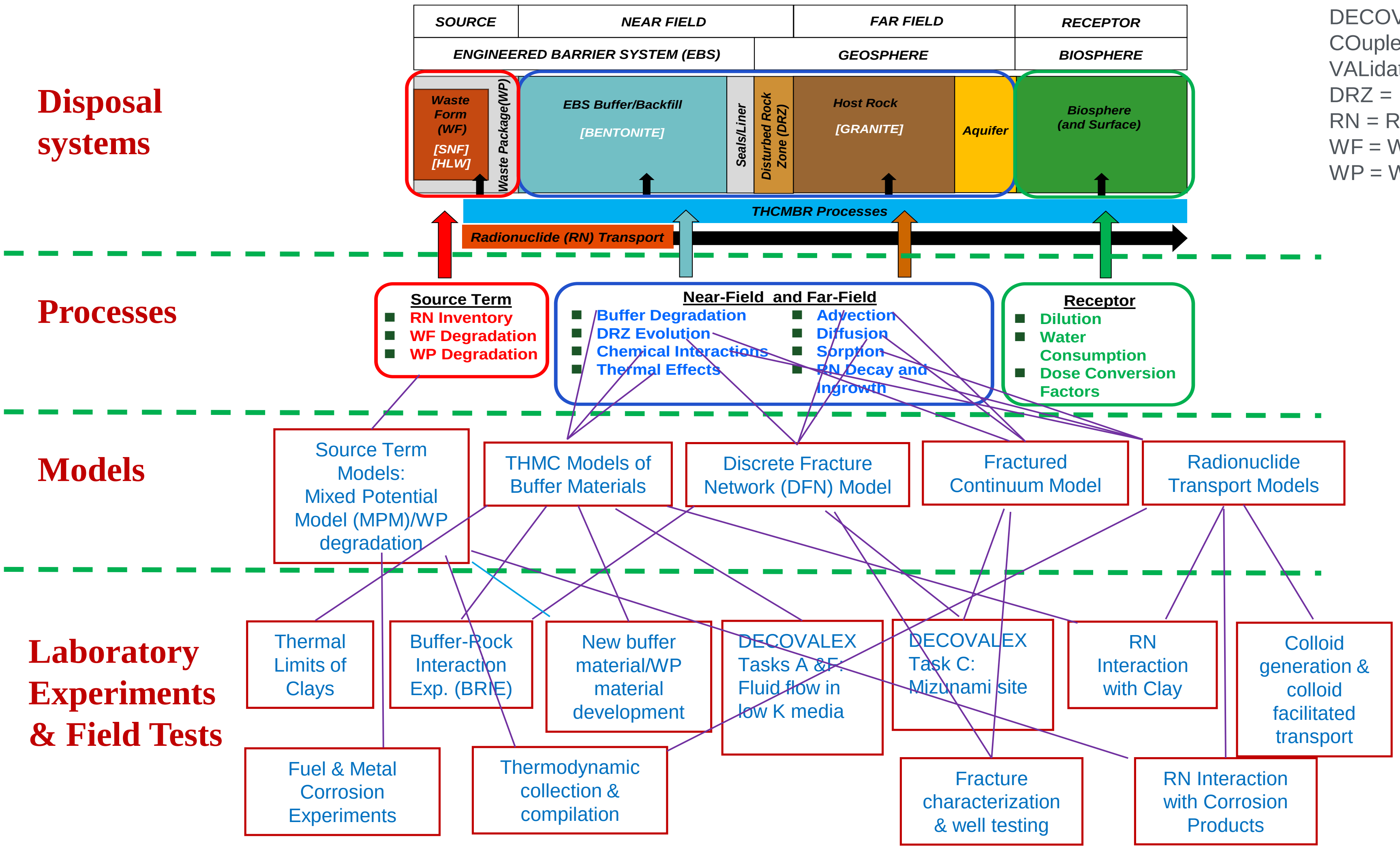
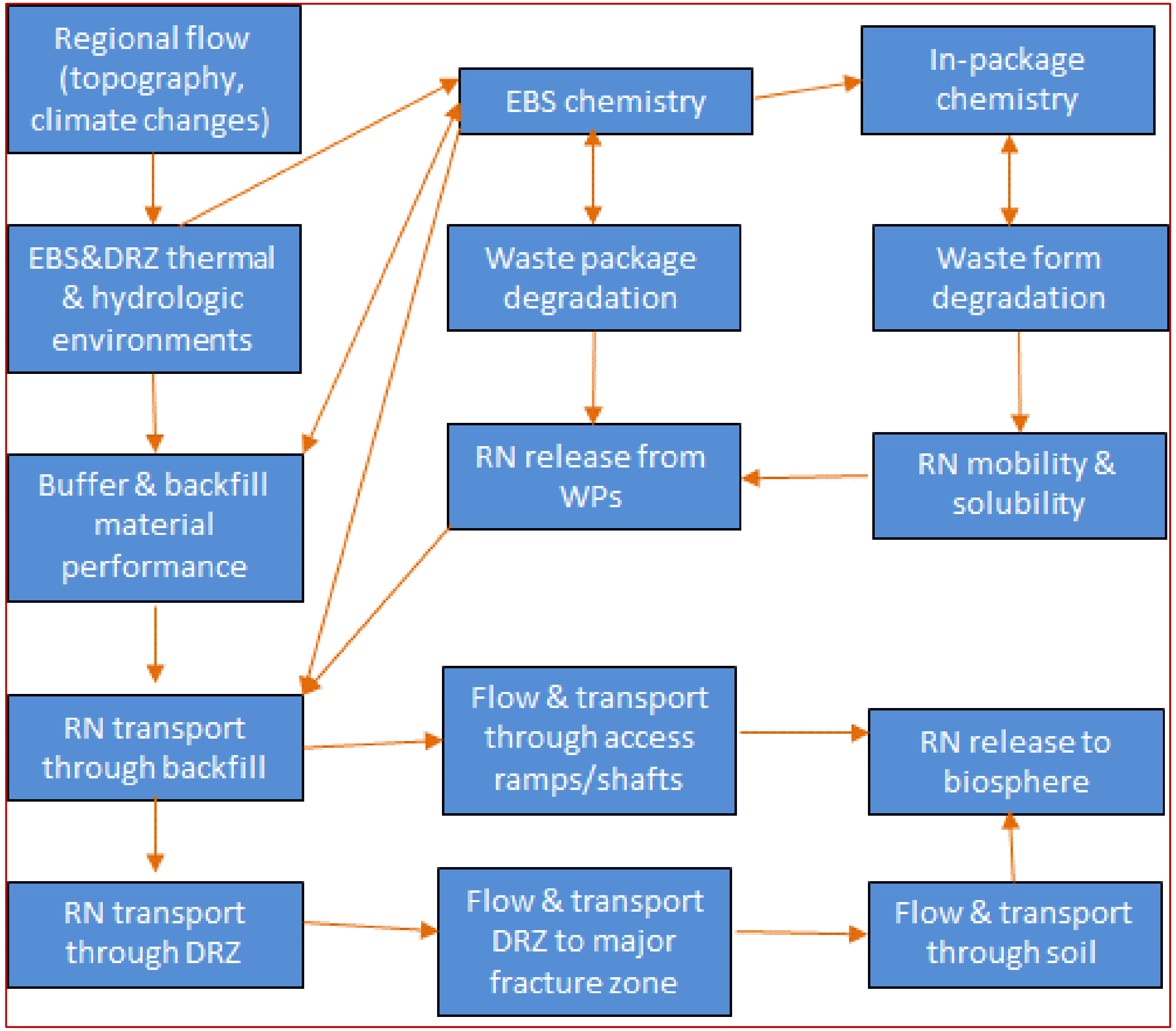
SAND2019-9033 R

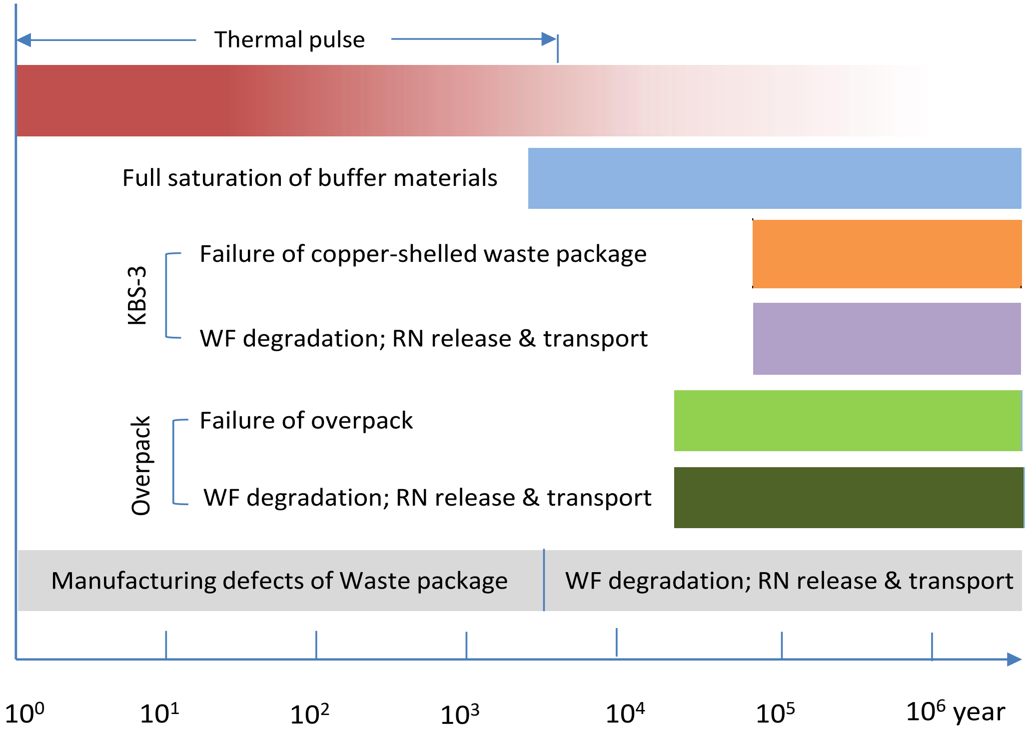
# Integrated experimental & modeling activities for used fuel disposition in crystalline rocks




DECOVELAX = DEvelopment of COupled models and their VALidation against EXperiments
DRZ = Disturbed rock zone
RN = Radionuclide
WF = Waste form
WP = Waste package

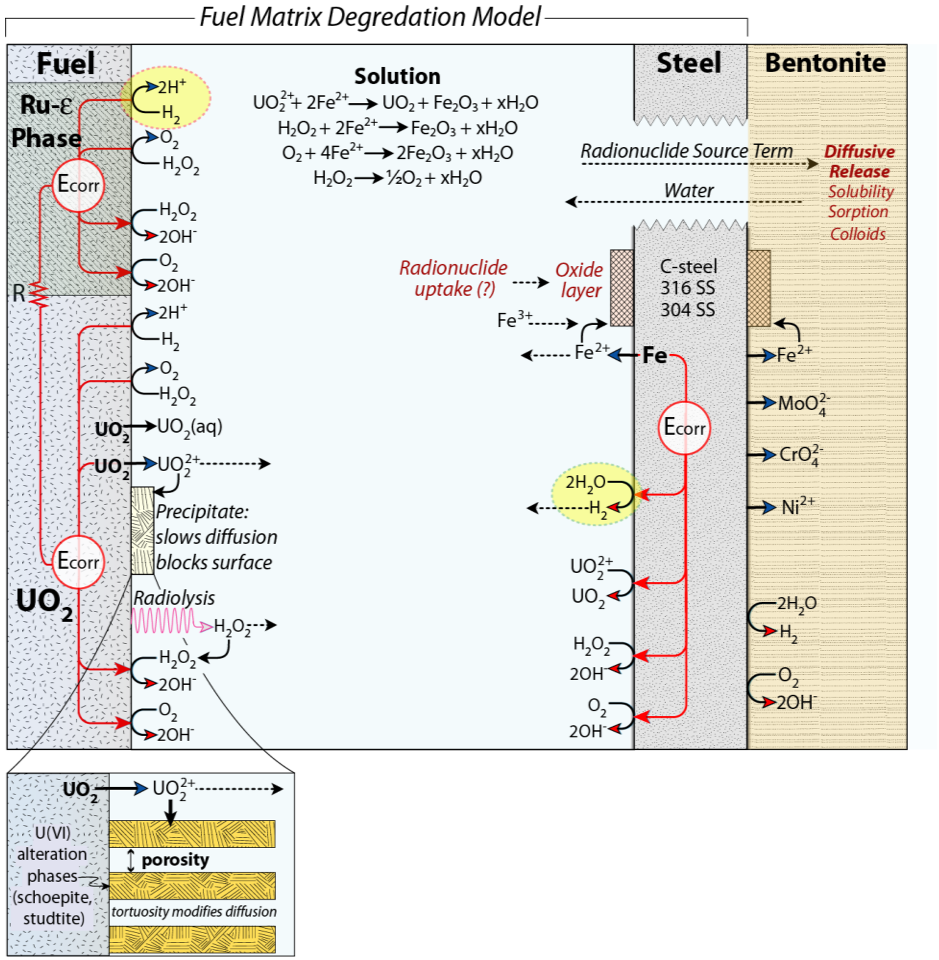
# State of knowledge of process models



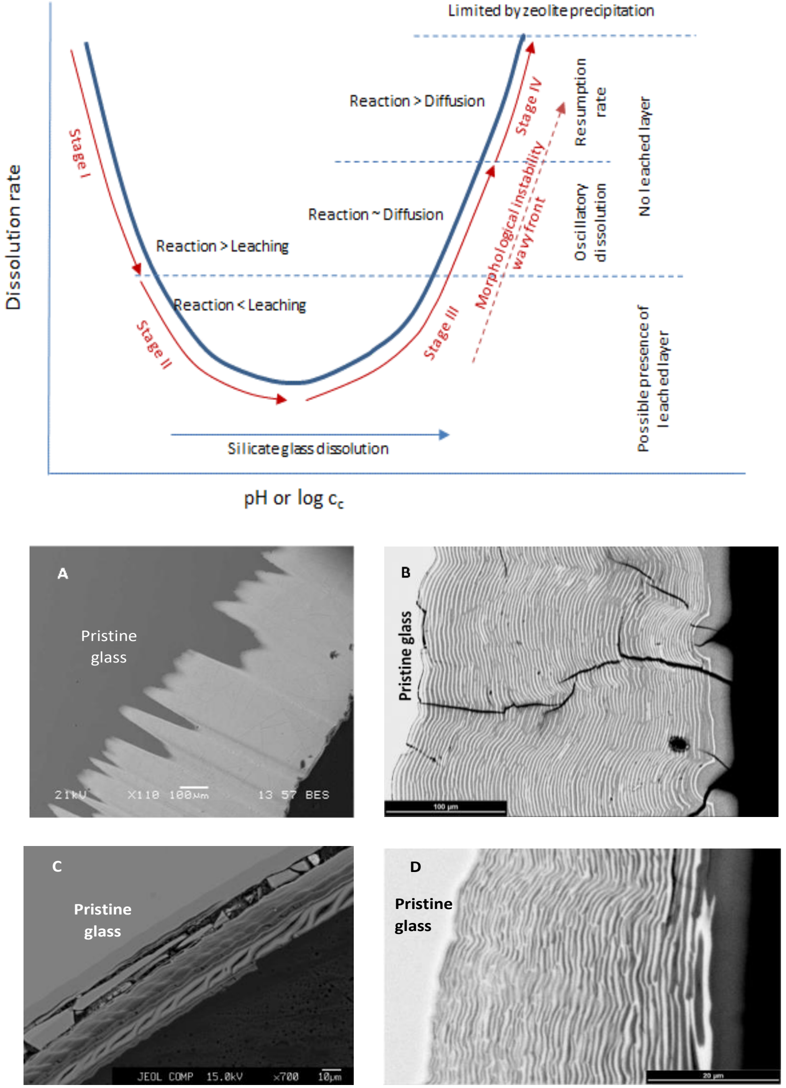




DRZ = Disturbed rock zone
RN = Radionuclide
THMC – Thermal-hydrologic-mechanical-chemical
WP = Waste package

# Waste form degradation

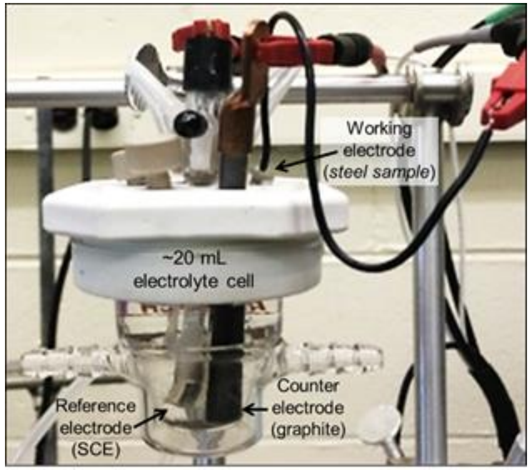



Fuel matrix degradation model
(Wang et al., 2020)



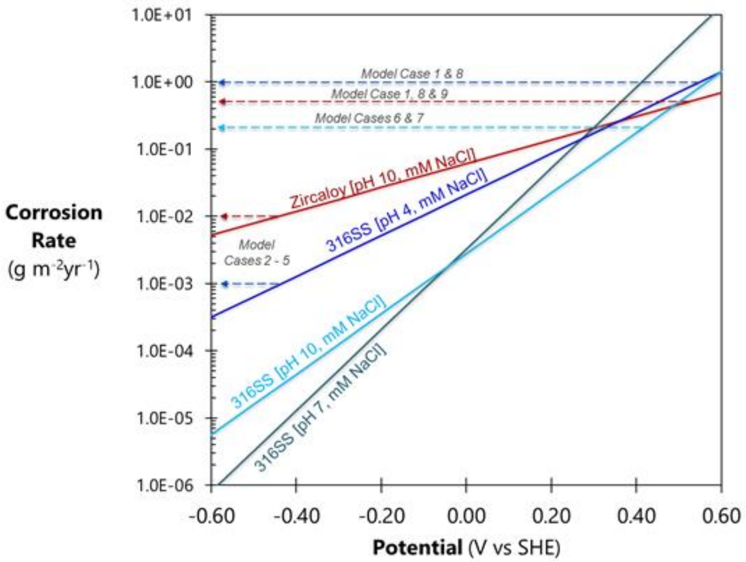

Nonlinear glass corrosion model
(Wang et al., 2016)

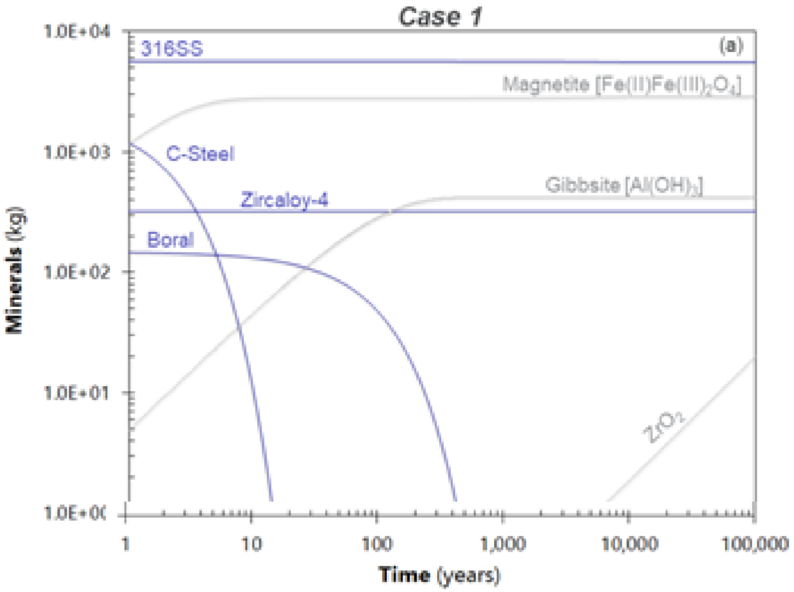
# Waste package degradation

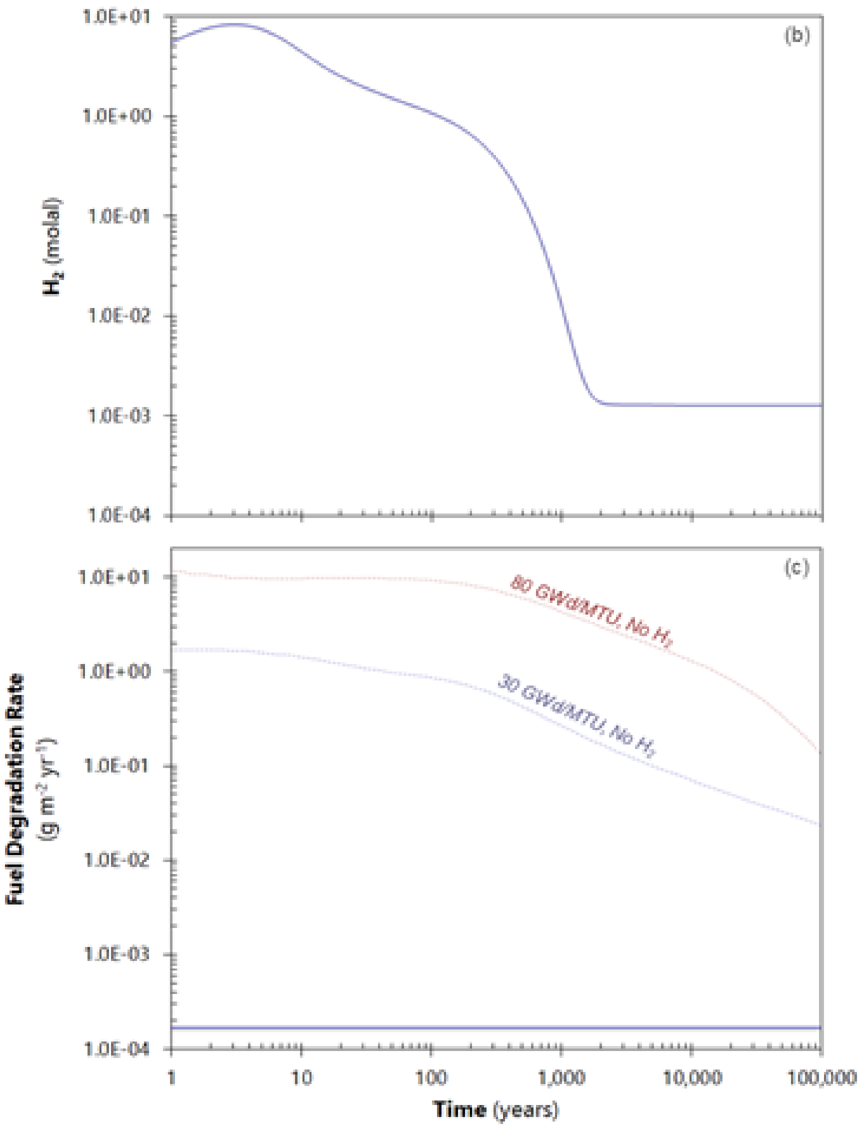



Three-electrode electrochemical cell

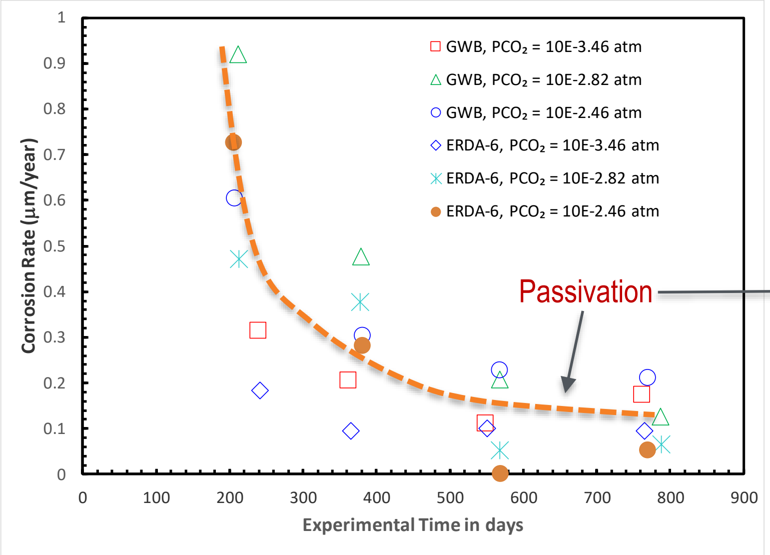
Wang et al. (2020)

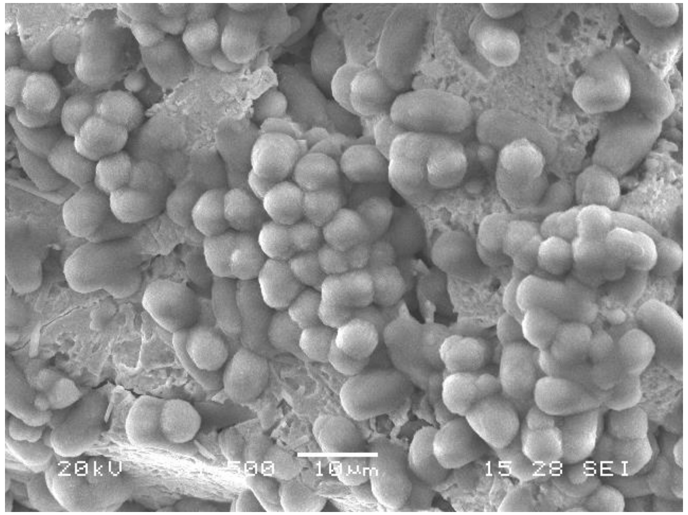


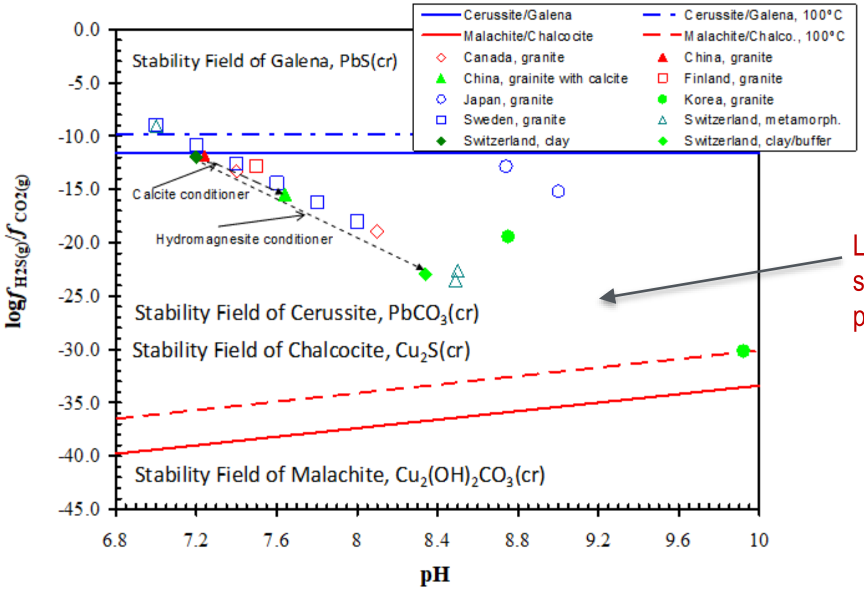



# Lead/lead-alloy as a corrosion-resistant outer layer packaging material



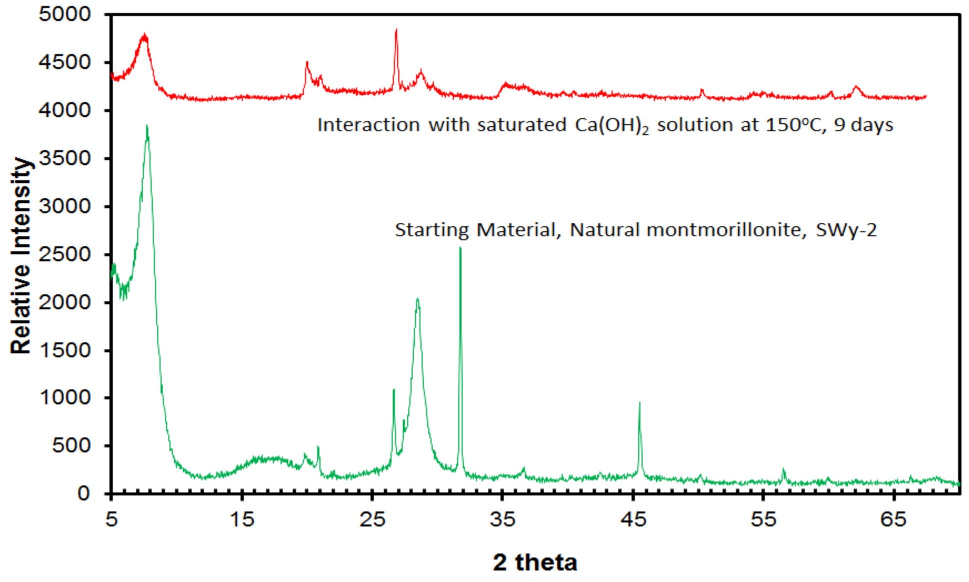




Lead/lead alloy is much more stable than copper in the presence of H2S.

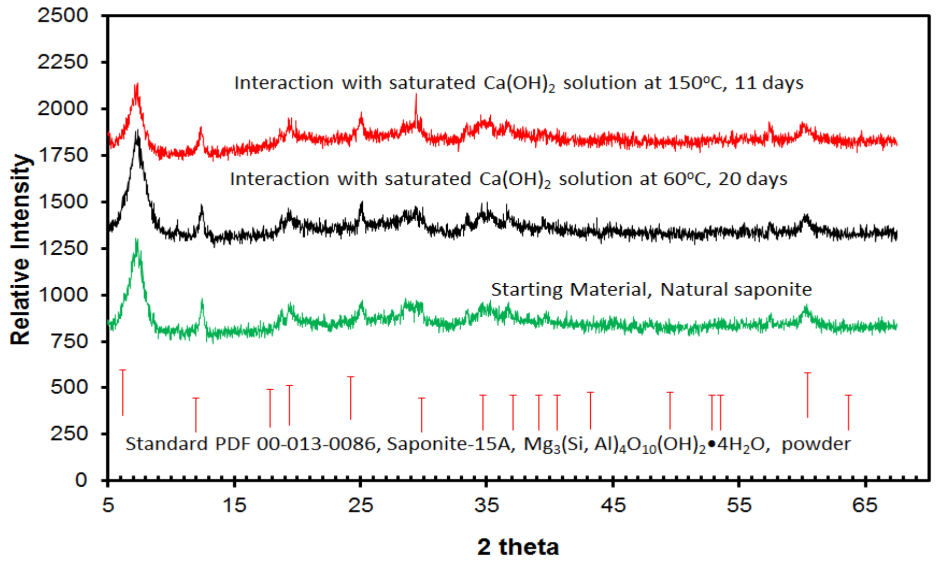
- Requirements
  - Longevity: >1000 years ✓
  - Avoid any detrimental impacts on other EBS materials. ✓
  - Retrievability ✓
  - Radiation shielding ✓
  - Reasonable structural strength (tensile stentgh 70 MPa for alloy) ✓
  - Availability ✓
- Lead
  - Good resistance in sulfide environments
  - $0.87/lb
  - RCRA: Already present as fission product

# Development of next-generation buffer materials for harsh environments

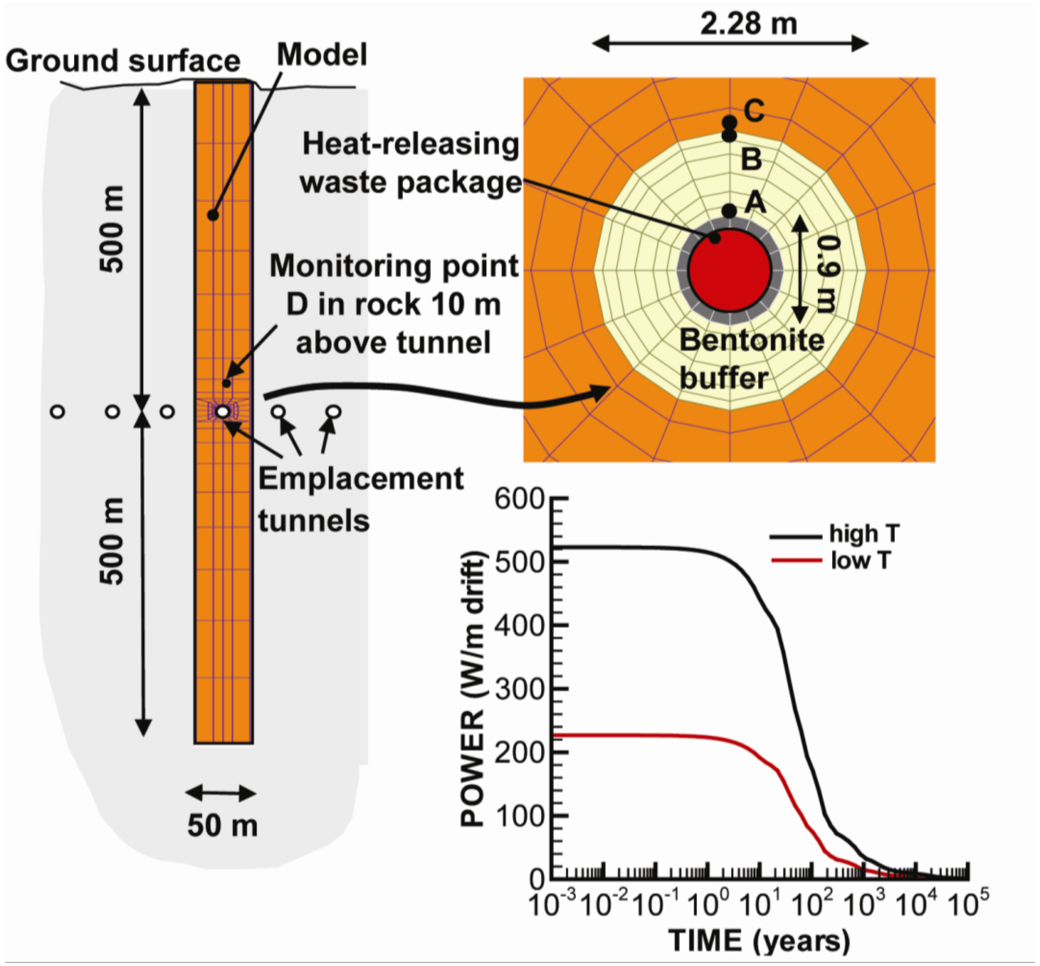


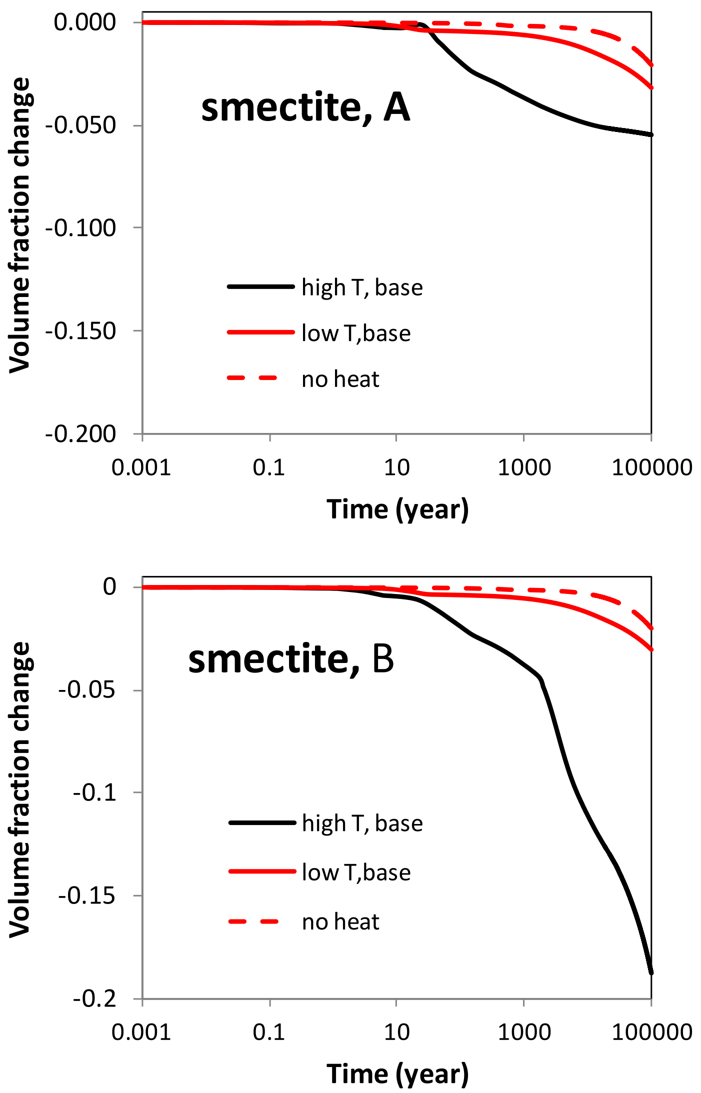

Leverage materials science and engineering for engineered material development.

Saponite is more stable than Na-montmorillonite in alkaline and high temperature environments.



# Thermal-hydrologic-mechanical-chemical (THMC) modeling of buffer materials



# Radionuclide transport through buffer materials: Pu interaction with goethite and clay

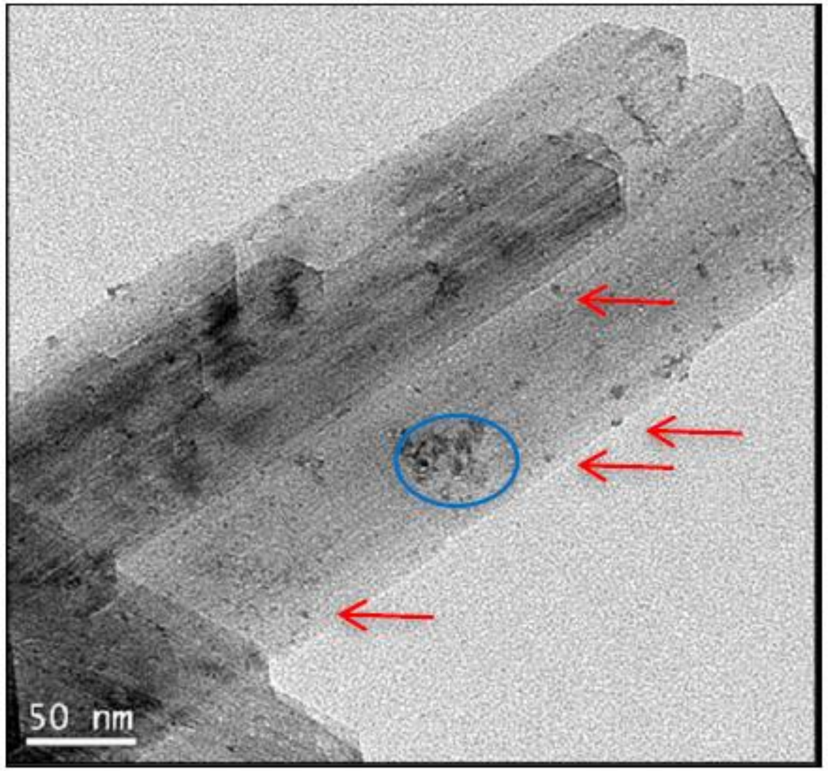



**Figure 2-11.** Both $PuO_2$ aggregates (blue) and dispersed $Pu_4O_7$ (red) on the goethite surface were observed at 25°C in high concentration samples. 8900 ppm Pu on goethite.

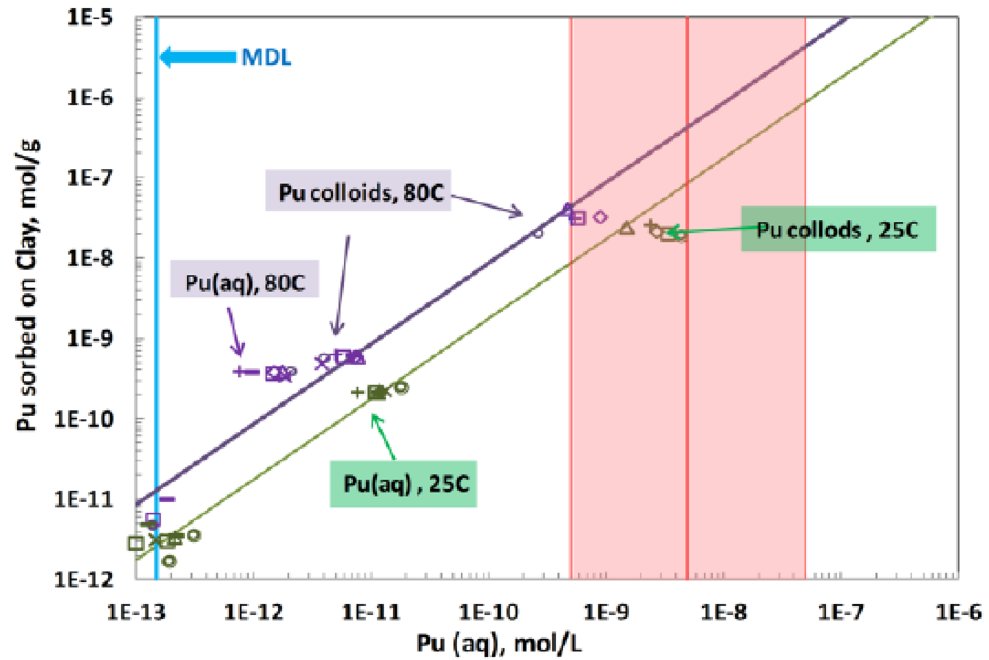
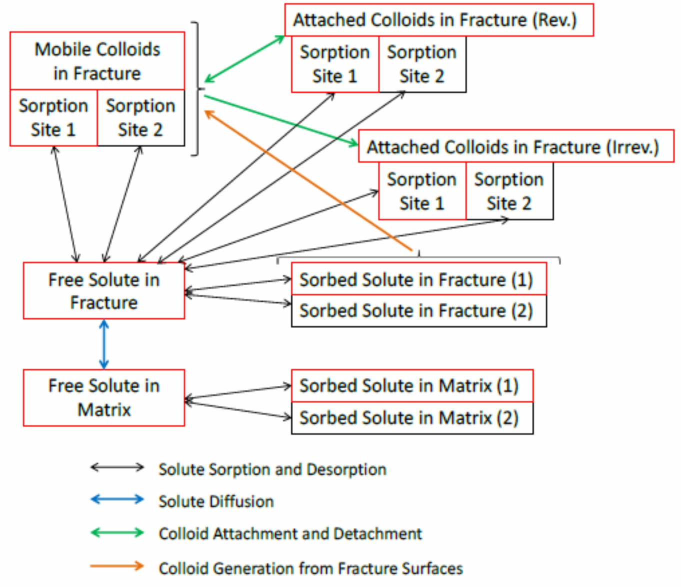


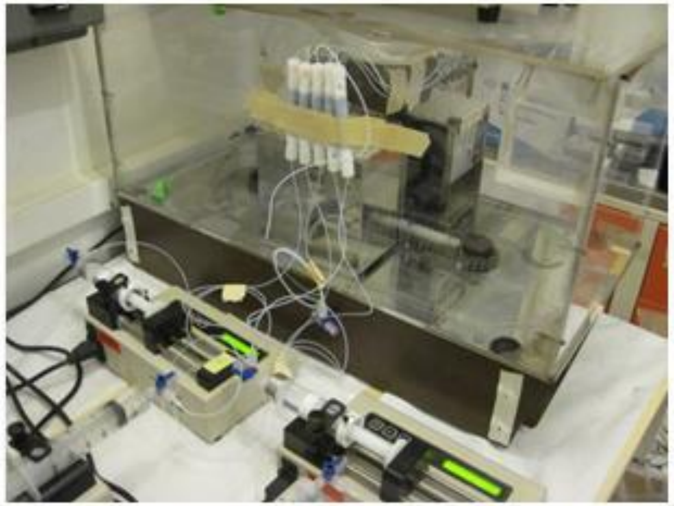

**Figure 3-7.** Summary of Pu sorption data at 25°C (green points) and 80°C(purple points). Shift between the 25 and 80°C isotherm is indicative of increasing Kd with temperature.. Shaded zone is the reported total Pu concentration in equilibrium with PuO2(am, hyd) at pH 8. MDL – method detection limit.

Kersting et al. (2012)

# Colloid-facilitated transport model and buffer material erosion

Multiple site sorption model



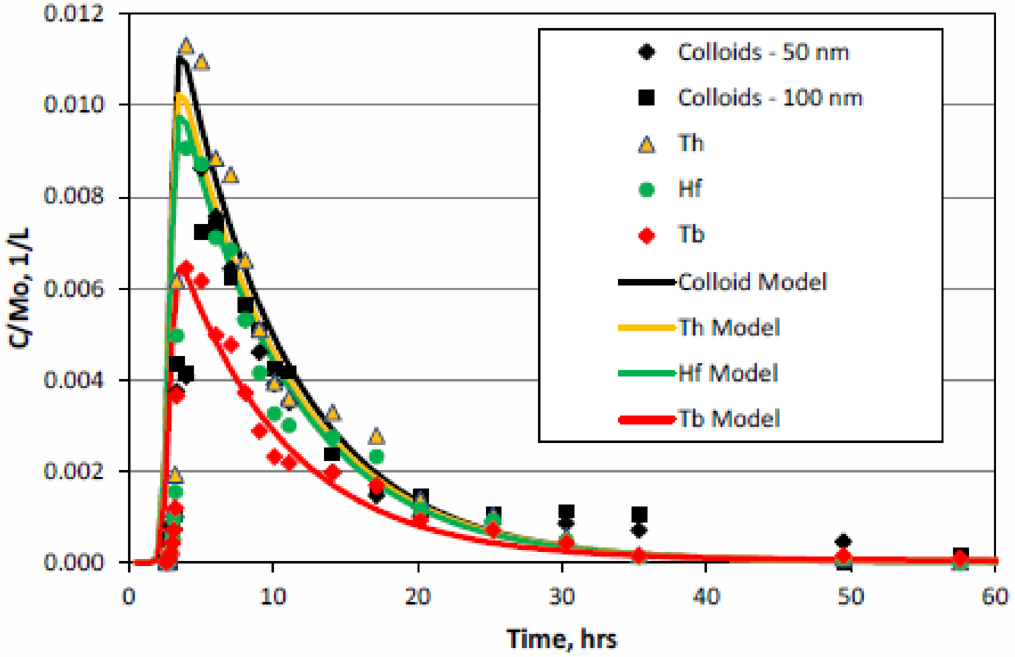
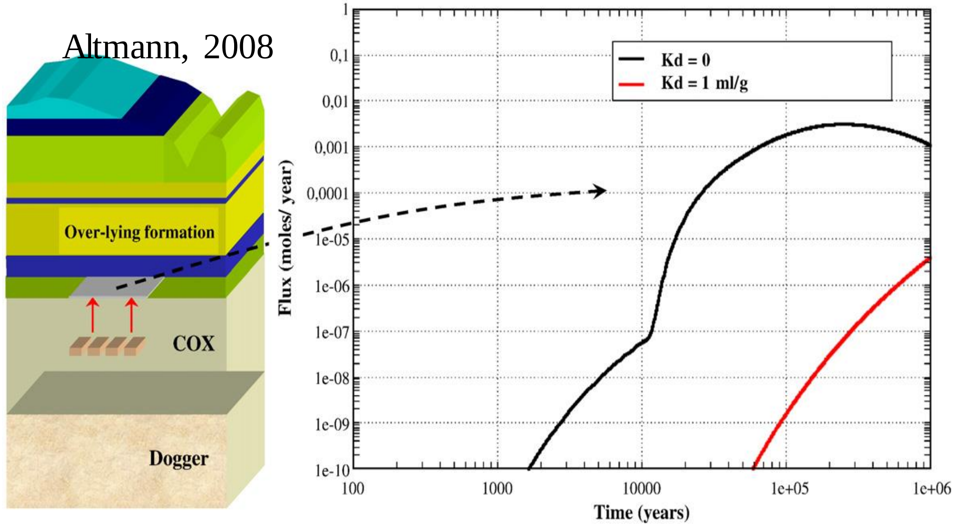



**Figure 2-11.** Model matches to the extraction breakthrough curves of test 08-01.

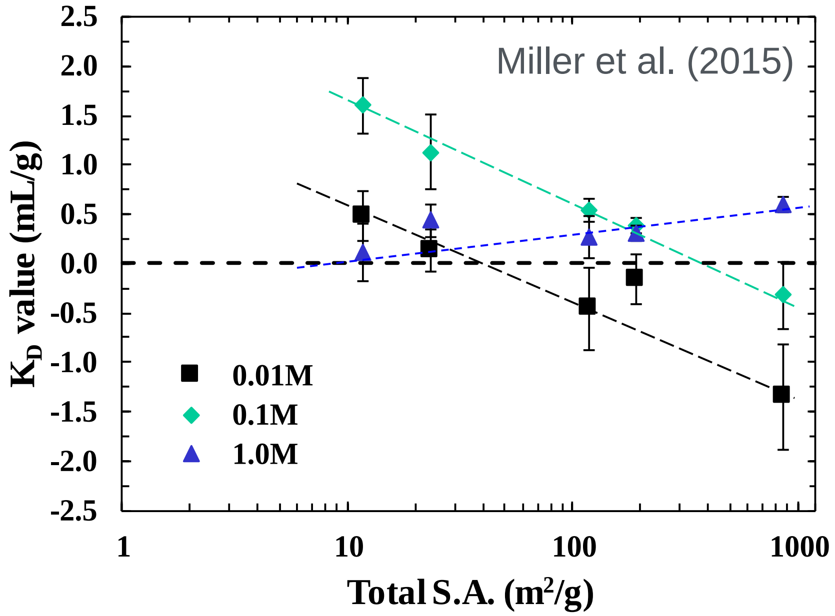
Multiple column experiments for interrogating radionuclide sorption parameters

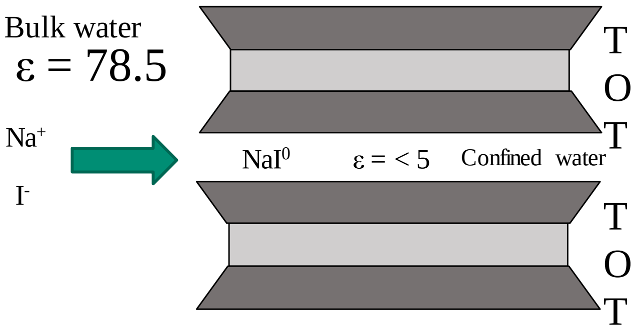
Reimus et al. (2017)

# Iodine-129 interaction with clays



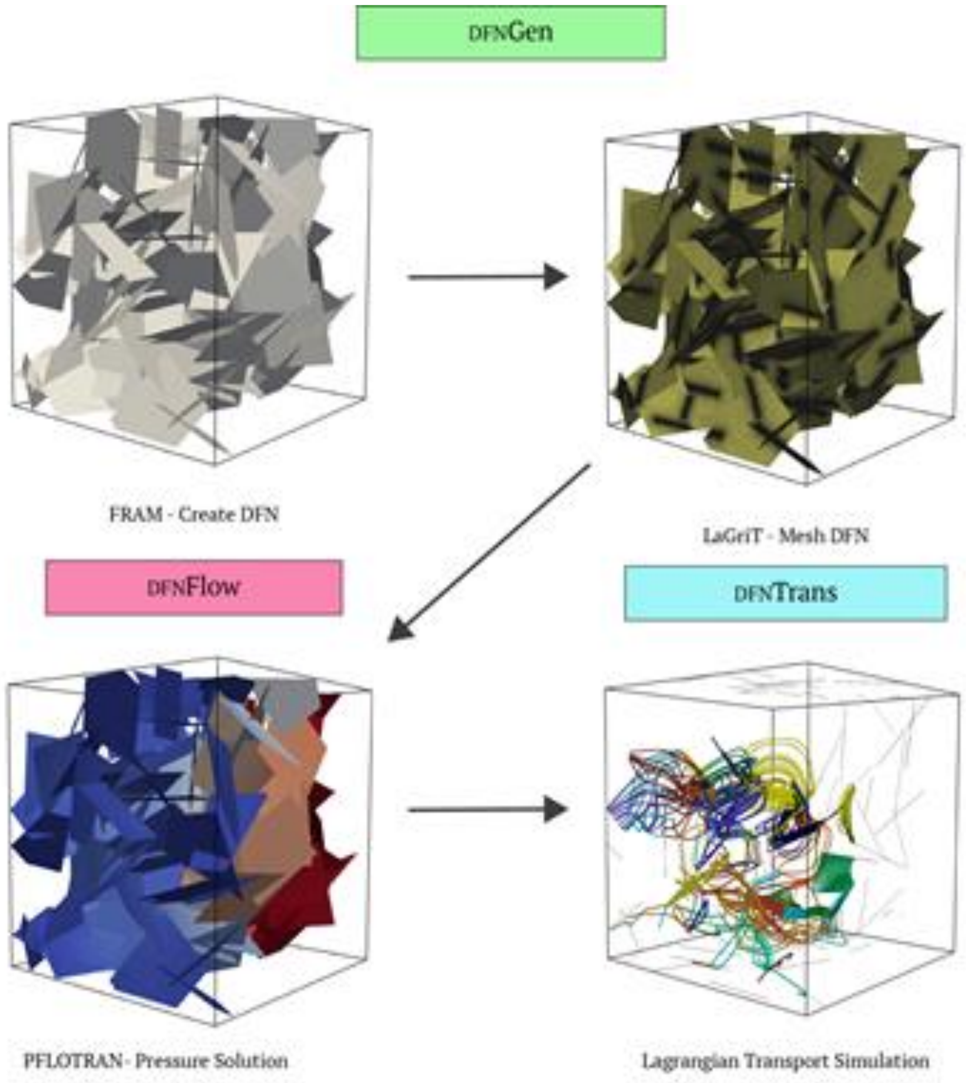

| Clay Mineral | Column $K_D$ Value (mL/g) | Batch $K_D$ Value (mL/g) | Ref. |
|---|---|---|---|
| Opalinus (Illite) | 0.008-0.02 | | Van Loon et al., 2003 |
| Montmorillonite | 0.57 | | Sato et al., 1992 |
| Callovo-Oxfordian (Interstratified illite/smectite) | | 0.15-0.37 | Bazer-Bachi et al., 2006 |
| Illite | | 27.7 | Kaplan et al., 2000 |
| Montmorillonite | | -0.33 | Kaplan et al., 2000 |

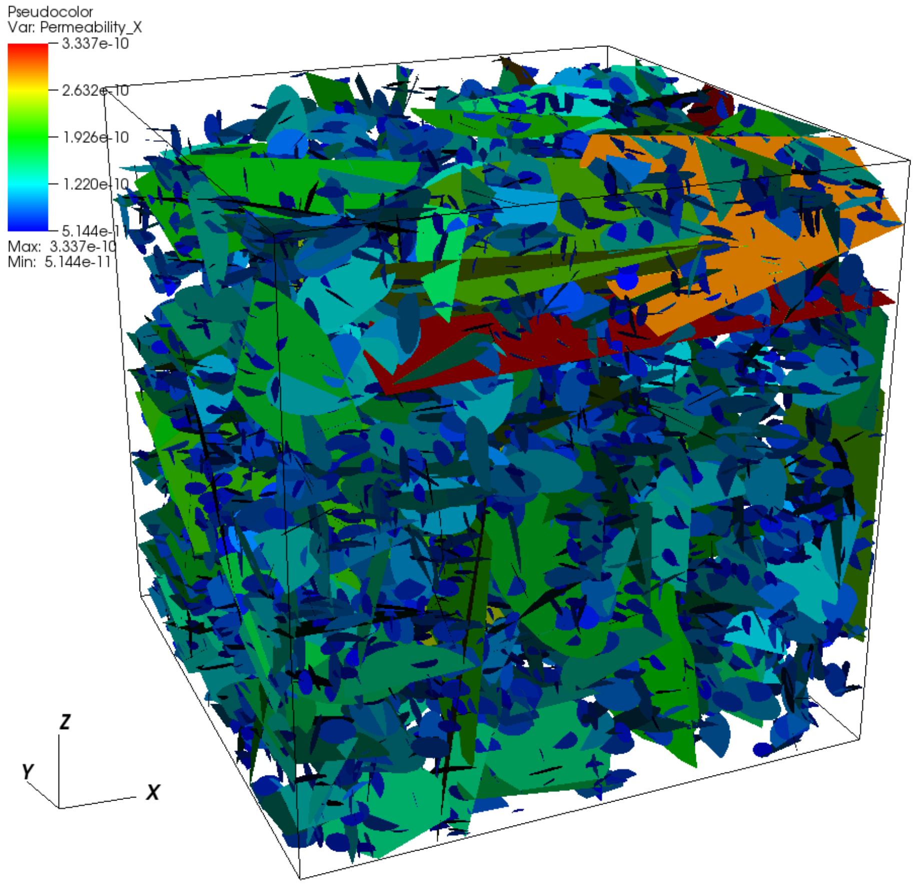



Iodide interacts with negatively charged clay interlayers through ion pairing induced by nanoconfinement.

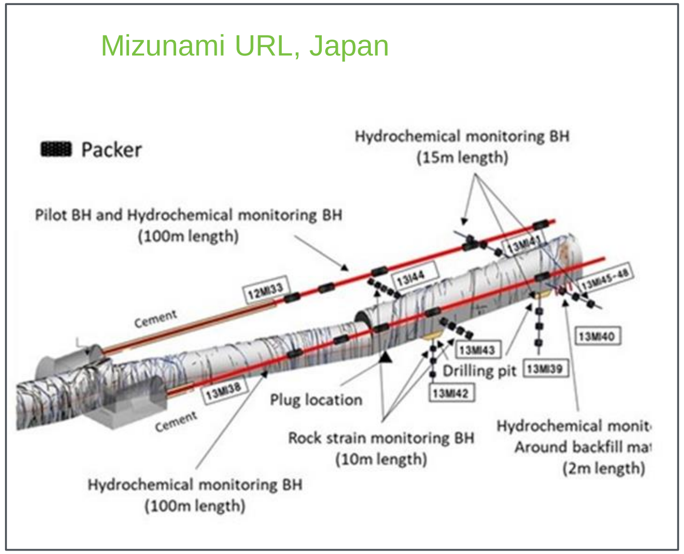
# Development of discrete fracture network model

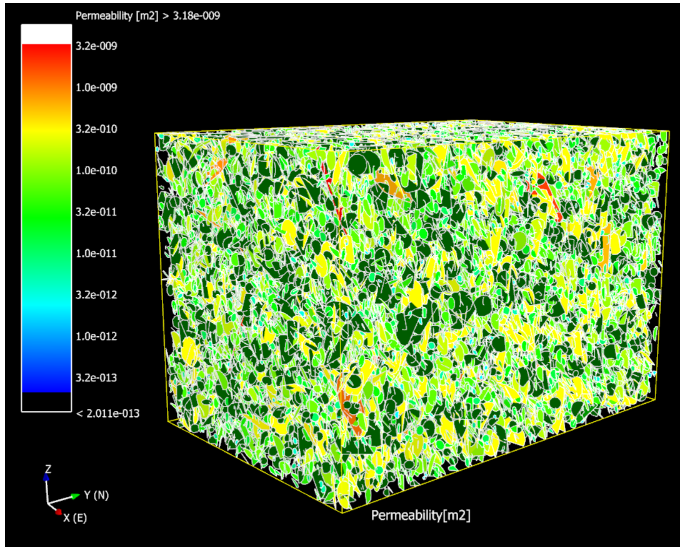


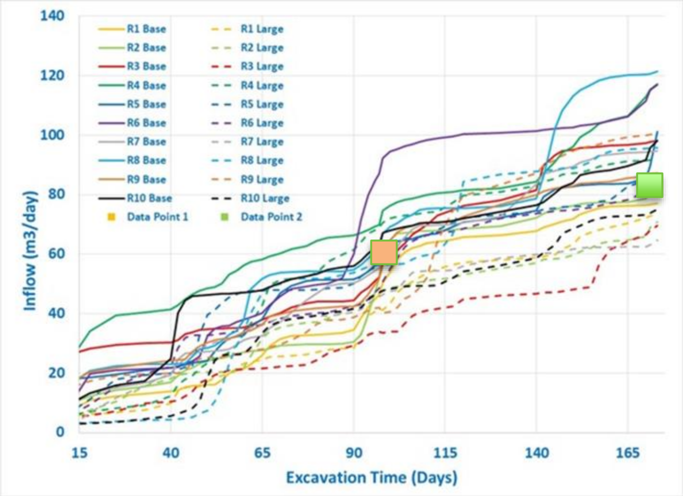



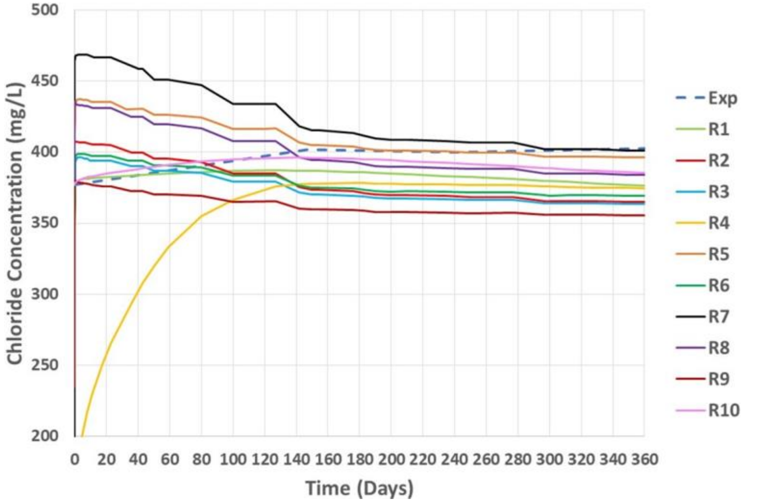

Hadgu et al. (2017)

# Development of a workflow for synthesizing field data into a fracture network model



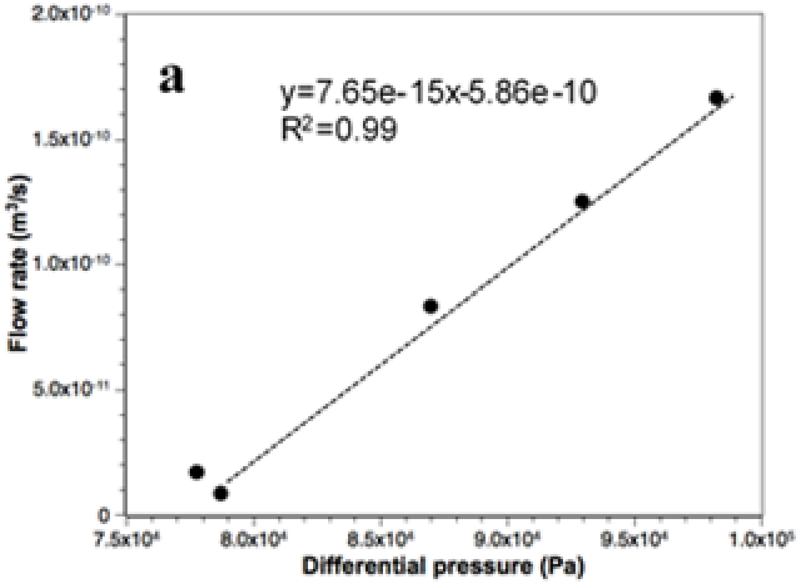



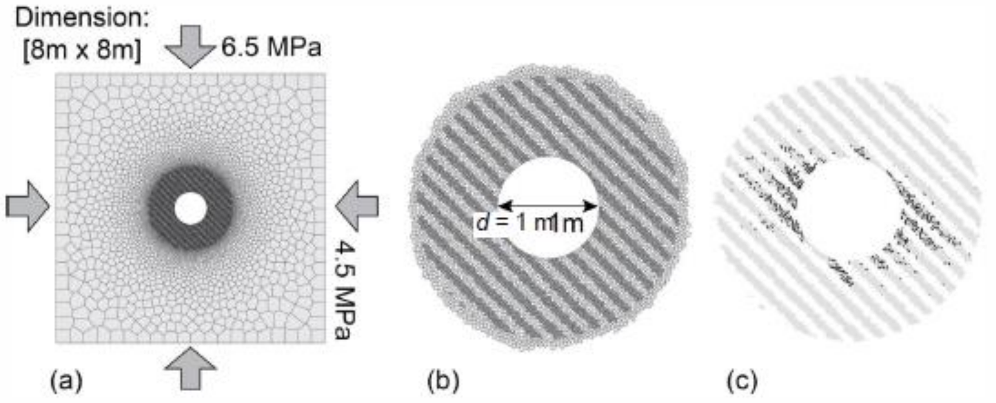

- It is important to condition fracture network generation on actual fracture distribution (location, size) in tunnel and borehole.
- Statistical stability of fracture networks?

# Technology for site characterization and monitoring: Disturbed rock zone (DRZ) characterization

Dual-sample triaxial rock testing system

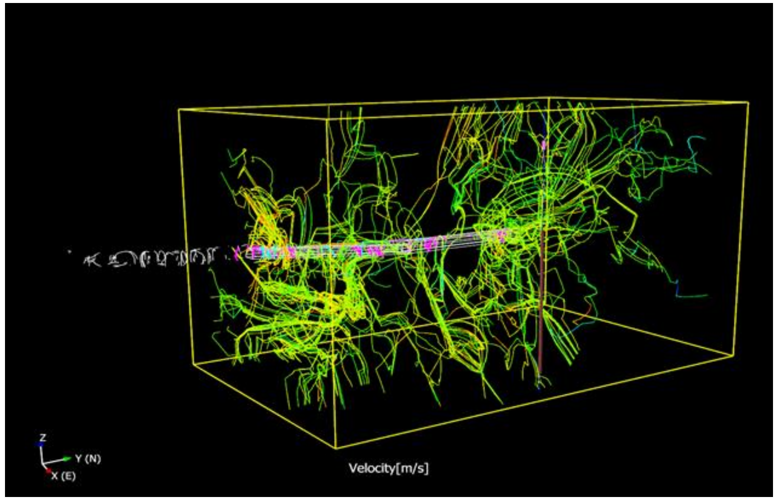


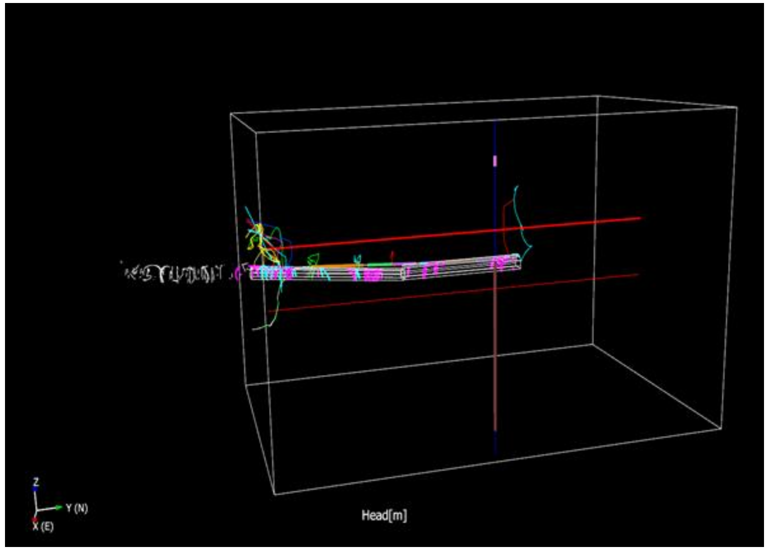

Granite core samples from Grimsel, Switzerland




Rigid-body-spring network model for simulating fracture patterns

# Fracture characterization and field monitoring

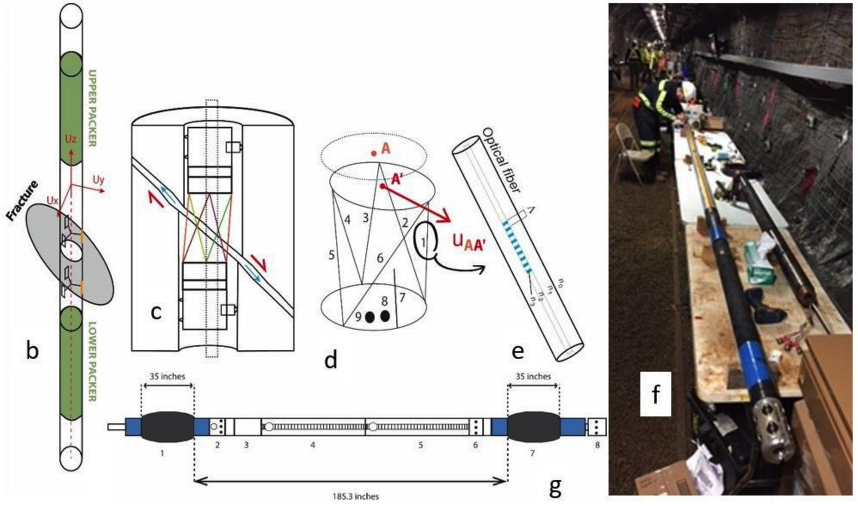



500 particles evenly distributed within the tunnel at time 0.

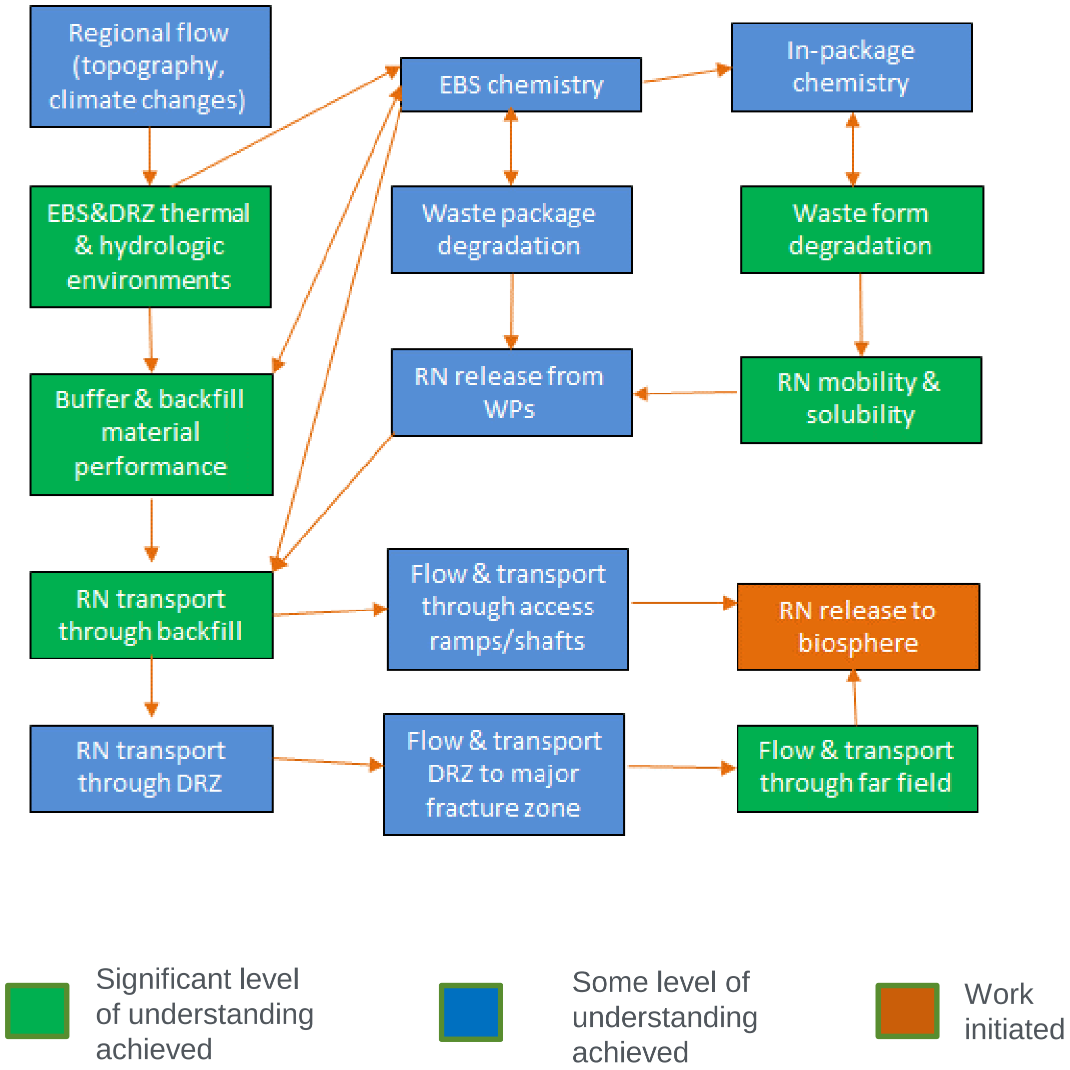
| Relization | 12MI33 | Upper Well | Lower Well |
|---|---|---|---|
| 5 | 1 | 3 | |
| 7 | | 9 | |
| 10 | | 5 | |
| 12 | | 1 | |
| 13 | 2 | | |
| 15 | | 1 | |
| 17 | | 1 | |
| 21 | | 1 | 1 |
| 23 | 2 | | |
| 24 | 1 | | |
| 25 | | 1 | |

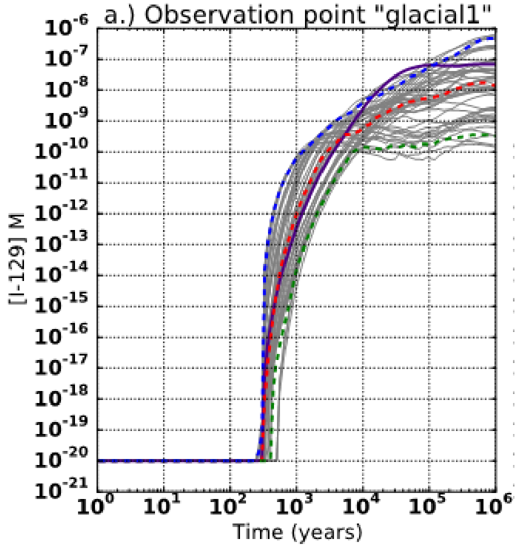
- The challenge of groundwater monitoring in fractured rocks is to design a system that captures sufficient number of particles.
- Technologically, this challenge is related to the ability for fracture characterization.
- High-resolution geophysical techniques are highly desirable.

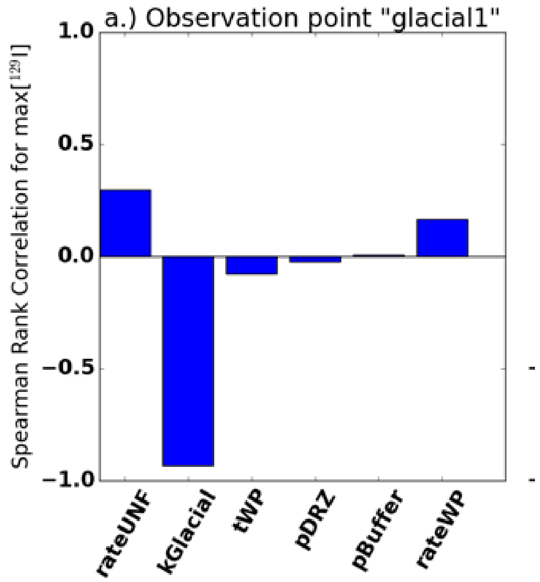



Step-rate Injection Method for Fracture In-situ Properties (SIMFIP) system

# Current status of process models and total system integration



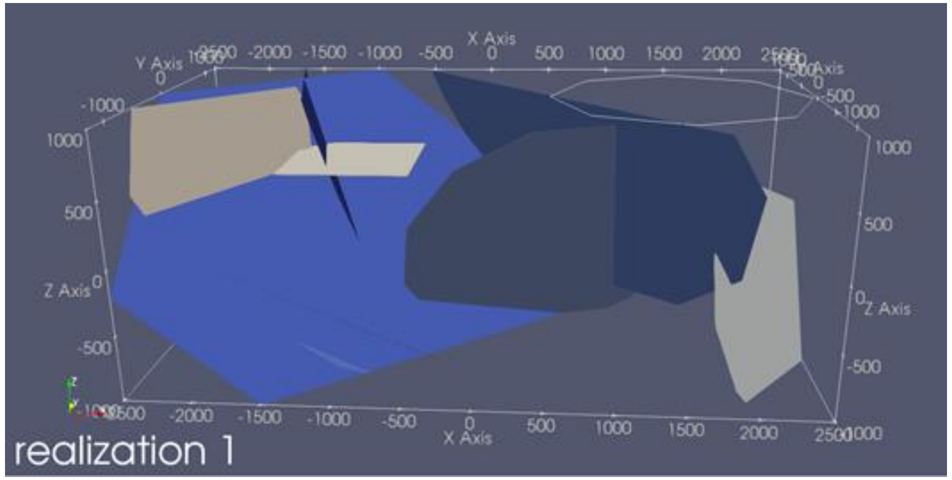



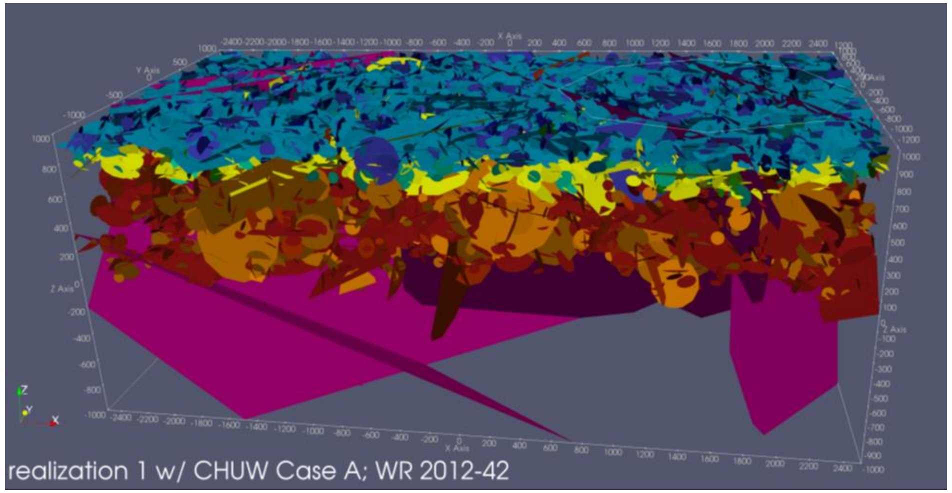
# Next steps

- Develop a sensible GDSA model for sensitivity analyses.
  - Provide a minimum set of process models to GDSA
- Move model development more towards model validation with real data.
- Develop reduced order models for incorporation into the GDSA model.
- Continue with buffer material development.
- Develop and refine engineered barrier system (EBS) models, especially waste package (WP) degradation models.

Towards a more realistic perception (then representation) of fluid flows in crystalline rocks: Crystalline rocks are generally quite impermeable.




Deterministic fracture zones




Stochastic fractures

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# Questions?