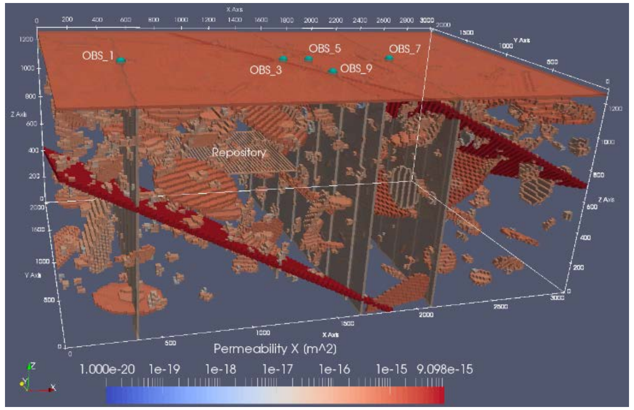

Overview of Activities Related to Disposal in Crystalline Host Rock

Chris Camphouse, Emily Stein, and Yifeng Wang

Sandia National Laboratories

U.S. NWTRB Meeting

May 21, 2024

Knoxville, Tennessee

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Spent Fuel and Waste Science and Technology (SFWST)

Outline

- **Research and development (R&D) context**
- **Demonstration of safety assessment capabilities and methods**
- **Objectives and overview of R&D activities**

R&D Context

Disposal in Crystalline Host Rock

Crystalline host rock is one of the natural barrier systems studied in the Spent Fuel and Waste Disposition (SFWD), Disposal Research program.

Crystalline Advantages

- High mechanical stability
- Low permeability (if unfractured)
- Good thermal conductivity
- Widespread occurrence

Crystalline Challenges

- Potentially high reliance on engineered barrier (fracturing)
- Fractured media characterization
- Flow and transport
- Model validation

SKB Äspö Hard Rock Laboratory, Sweden

Crystalline R&D Priorities

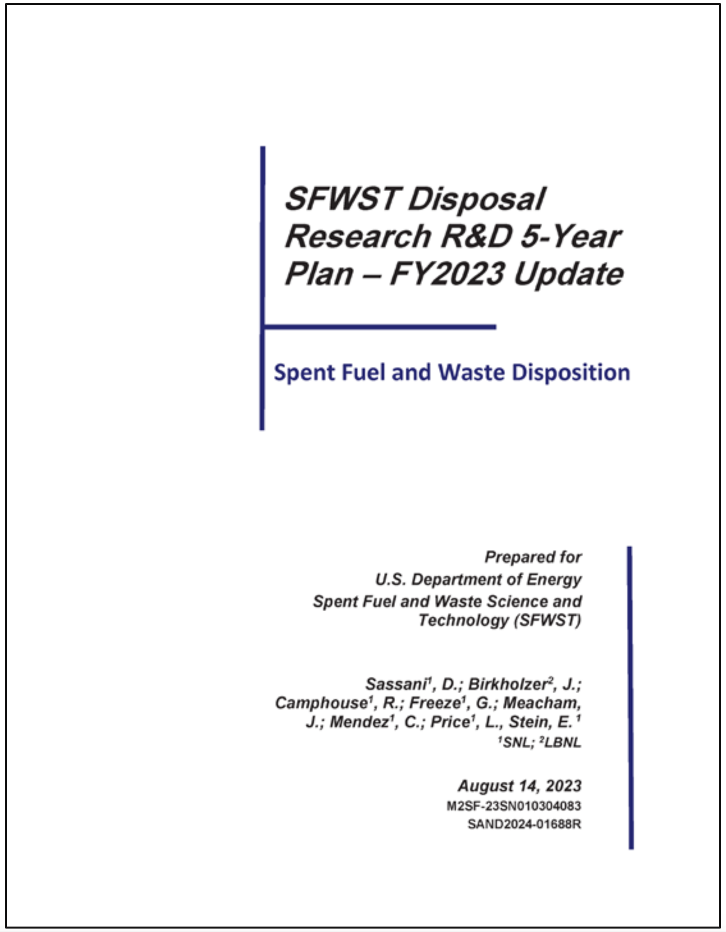
Crystalline R&D priorities are discussed in the 2023 revision to the Disposal Research 5-year plan.

R&D priorities:

- Improving statistical sampling and representation of fracture networks
- Investigating new generation of engineered barrier materials
- Improving representation of coupled thermal-hydrological-mechanical processes affecting fracture transmissivity

Reduced emphasis on discrete fracture network model development

- Focus is shifting from model development to model validation and demonstration with field data


SFWST Disposal Research R&D 5-Year Plan – FY2023 Update

Spent Fuel and Waste Disposition

Prepared for
U.S. Department of Energy
Spent Fuel and Waste Science and Technology (SFWST)

Sassani[1], D.; Birkholzer[2], J.; Camphouse[1], R.; Freeze[1], G.; Meacham, J.; Mendez[1], C.; Price[1], L., Stein, E.[1]
[1]SNL; [2]LBNL

August 14, 2023
M2SF-23SN010304083
SAND2024-01688R

International Collaborations

International collaborations are a significant component of Crystalline R&D.

These collaborations are important because they:

- Provide first-hand access to decades of experience from international partners
- Provide access to experimental data from past and ongoing in-situ tests
- Provide a framework for active peer-to-peer research participation in complementary international groups
- Enable joint development of experiments in international Underground Research Laboratories (URLs) not available in the Unites States
- Leverage substantial international investment in research facilities

International Collaboration Highlights

Grimsel Test Site URL

- FEBEX: 18-year full-scale in-situ heater test (100°C) focusing on bentonite backfill in crystalline host rock
- HotBENT: Test to assess bentonite buffer and near-field rock performance at high temperatures (175°C to 200°C)

SKB Task Force

- Flow and radionuclide migration processes in naturally fractured crystalline rock
- Coupled behaviors of the engineered barrier system

Swedish deep drilling characterization project (COSC)

- Fluid logging techniques to identify deep flowing fracture zones
- Subsurface stress state estimation

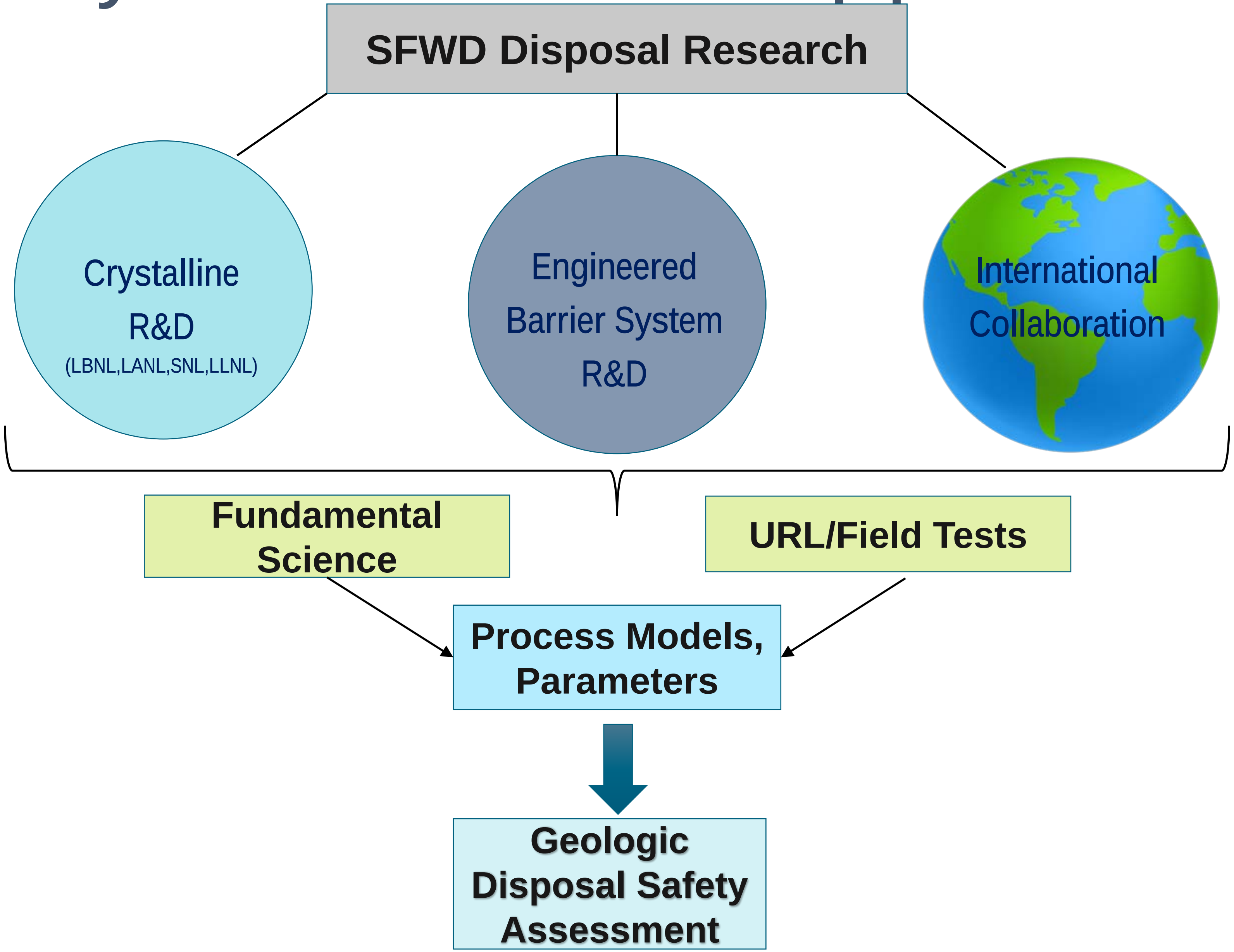
DECOVALEX-2023 Task G

- Representation of fracture mechanics when exposed to complex stress states

Nuclear Energy Agency Crystalline Club

- Exchanges of information and approaches for disposal in crystalline host rock

SFWD Crystalline R&D Approach



Demonstration of Safety Assessment Capabilities and Methods

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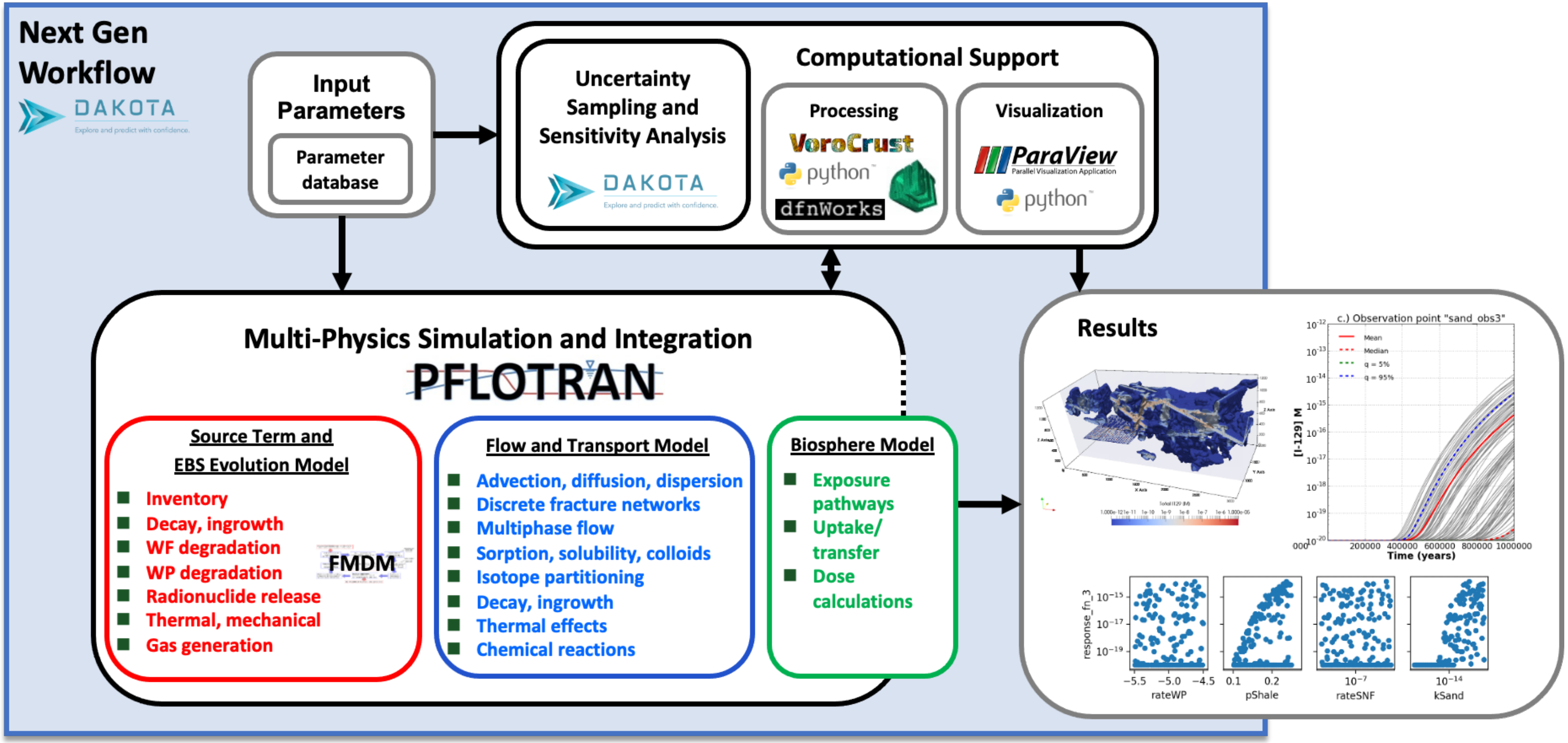
Geologic Disposal Safety Assessment (GDSA) Framework

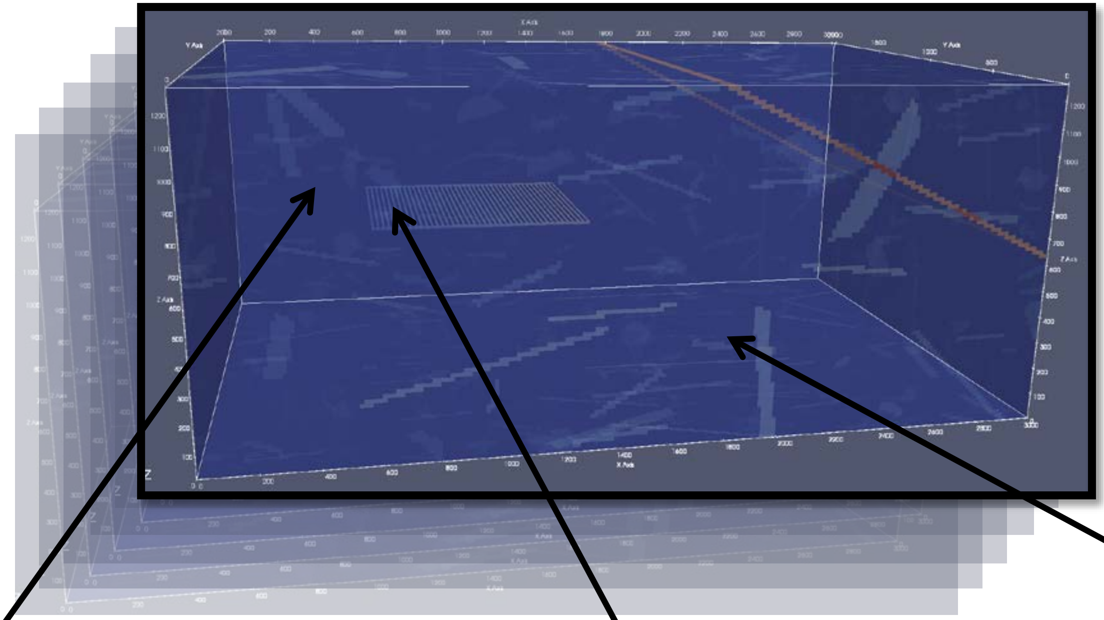


https://pa.sandia.gov/

Components of a Reference Case

DAKOTA
Explore and predict with confidence.

- Uncertainty quantification
- Sensitivity analysis



PFLOTRAN

- Coupled heat and fluid flow
- Waste package degradation
- Waste form dissolution
- Radioactive decay and ingrowth
- Solubility, sorption
- Advection, dispersion, diffusion

Source Terms

Engineered Barrier System

Natural Barrier System

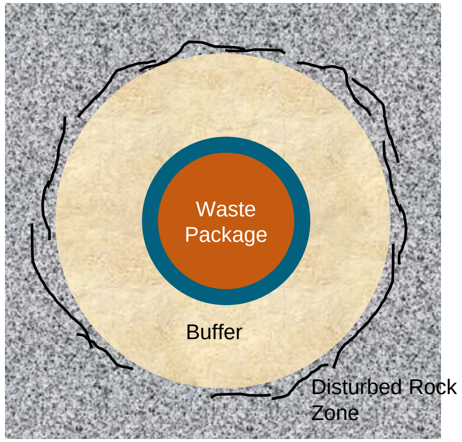
^{241}Am 4.3x10^2 y

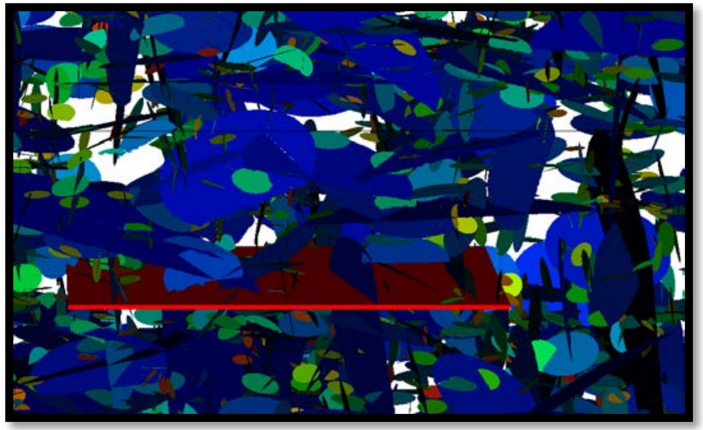
^{233}U 1.6x10^5 y

^{129}I 1.6x10^7 y

^{237}Np 2.1x10^6 y

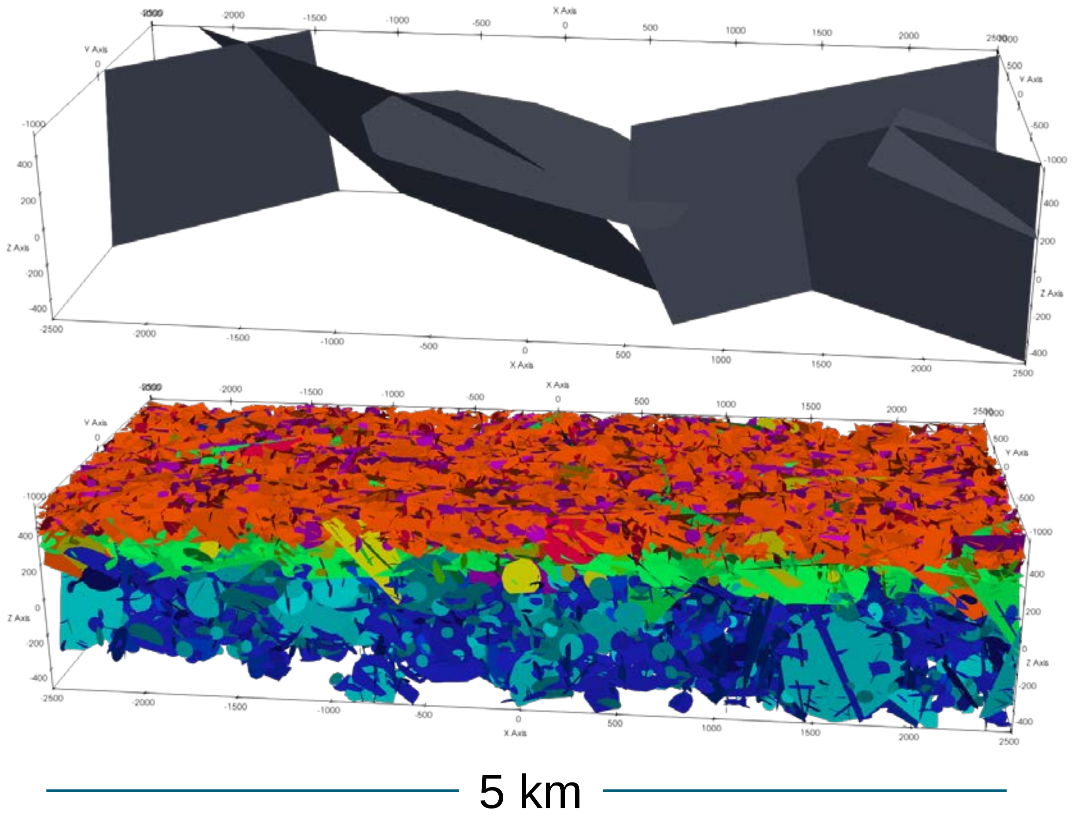
^{229}Th 7.3x10^3 y





Natural Barrier System

- **Outcropping or subcropping**
- **Sparsely fractured crystalline rock**
- **Low topographic slope**
- **Topographically controlled water table**
- **Consistent with international concepts**



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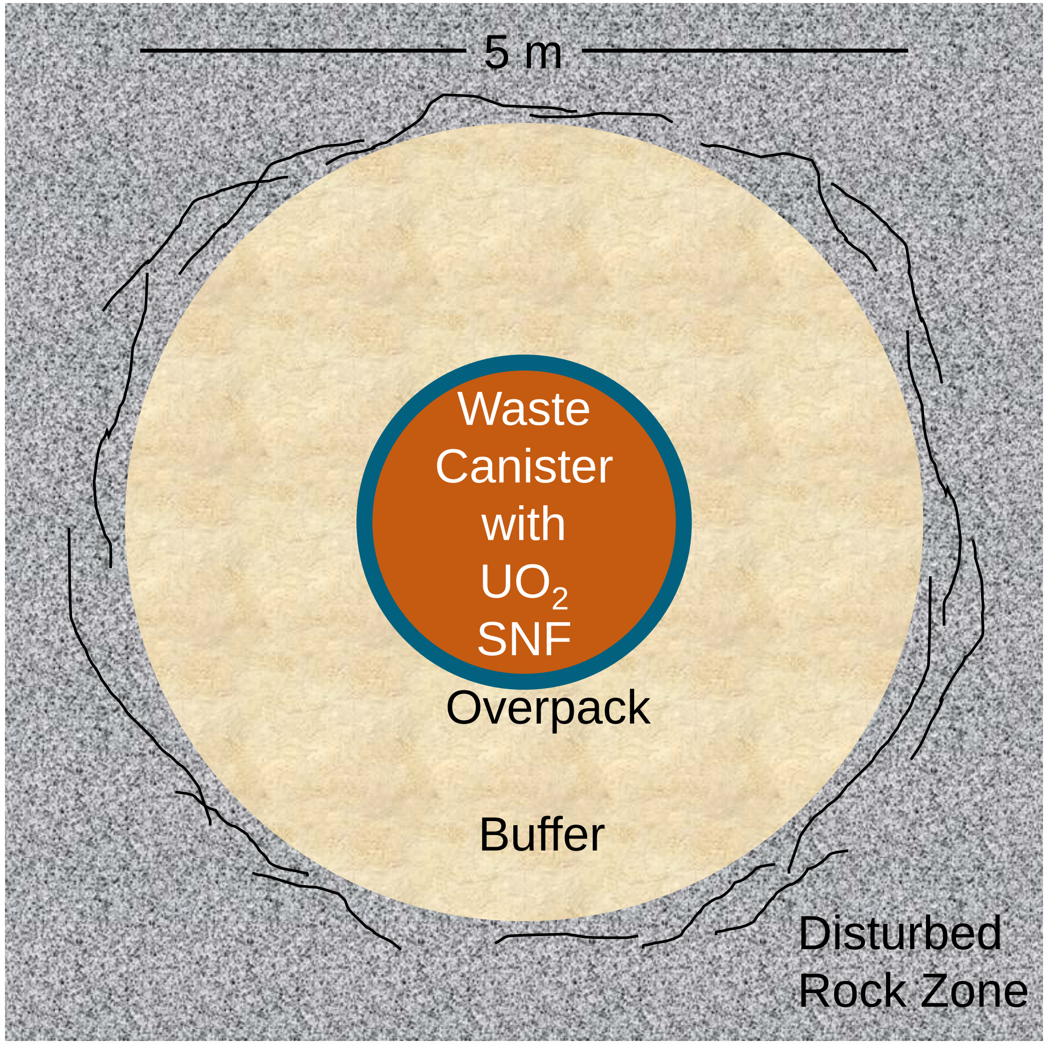
Engineered Barrier System

Rate-controlled degradation of

- UO_2 spent nuclear fuel (SNF)
- Waste package overpack

Radionuclide transport in

- Bentonite buffer
- Disturbed rock zone



Engineered Barrier System

Rate-controlled degradation of

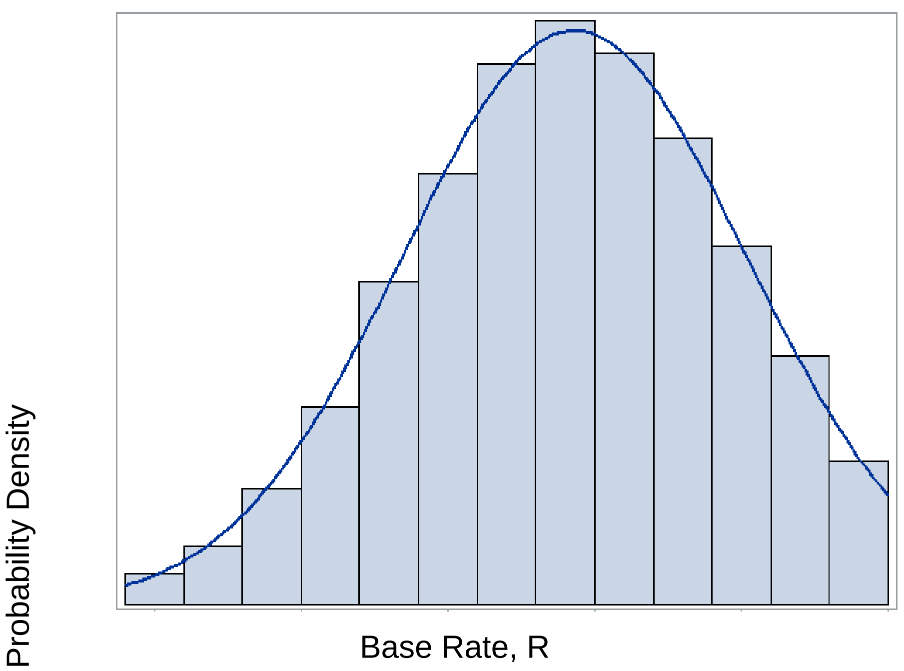
- UO_2 spent nuclear fuel (SNF)
- Waste package overpack

$$R_{eff} = R \cdot e^{C\left[\frac{1}{60℃} - \frac{1}{T(x,t)}\right]}$$

Radionuclide transport in

- Bentonite buffer
- (Disturbed rock zone)

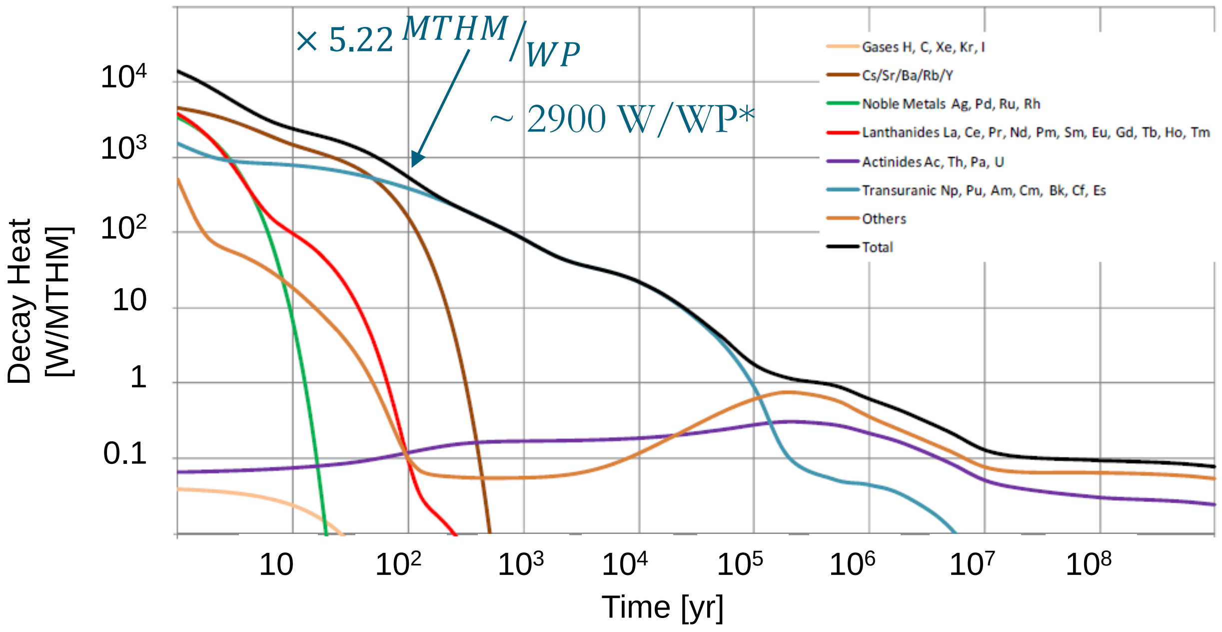
Bentonite erosion



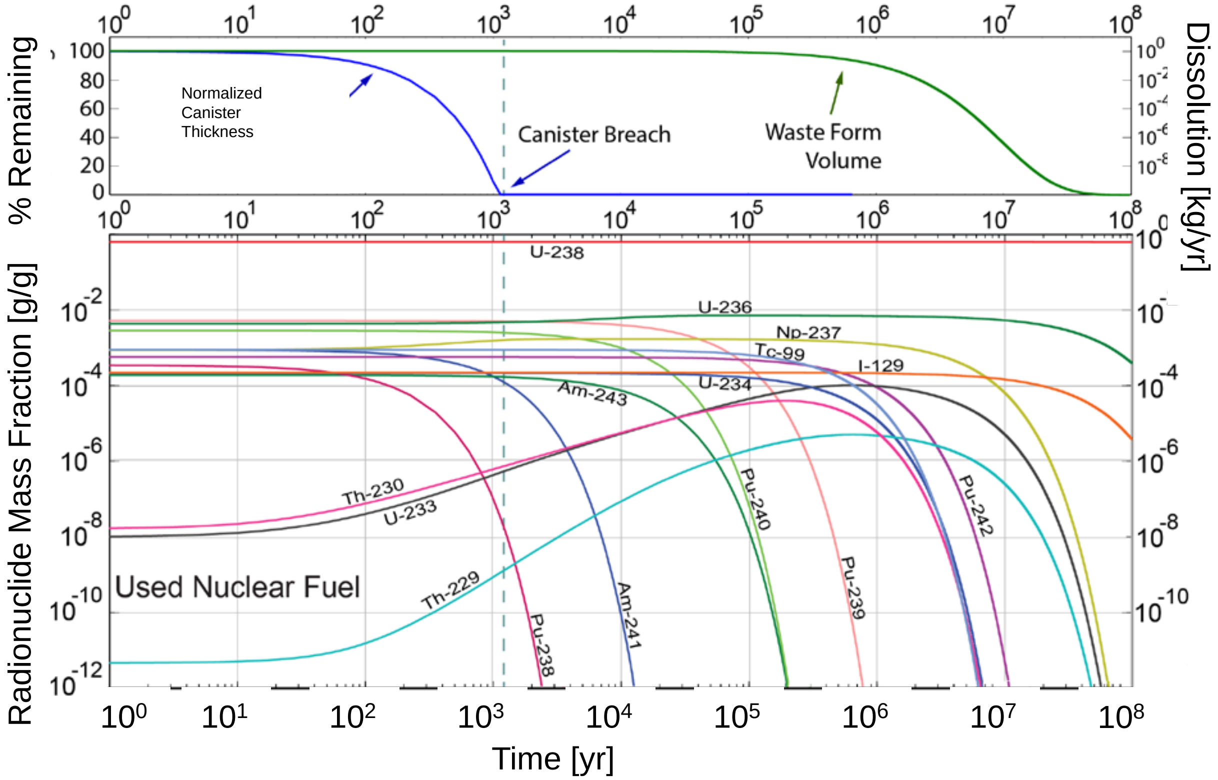
Heat and Radionuclide Source Terms

Assumptions

- 4.73 wt% ^{235}U enrichment
- 60 GWd/MT burn-up
- 100 yrs Out of Reactor



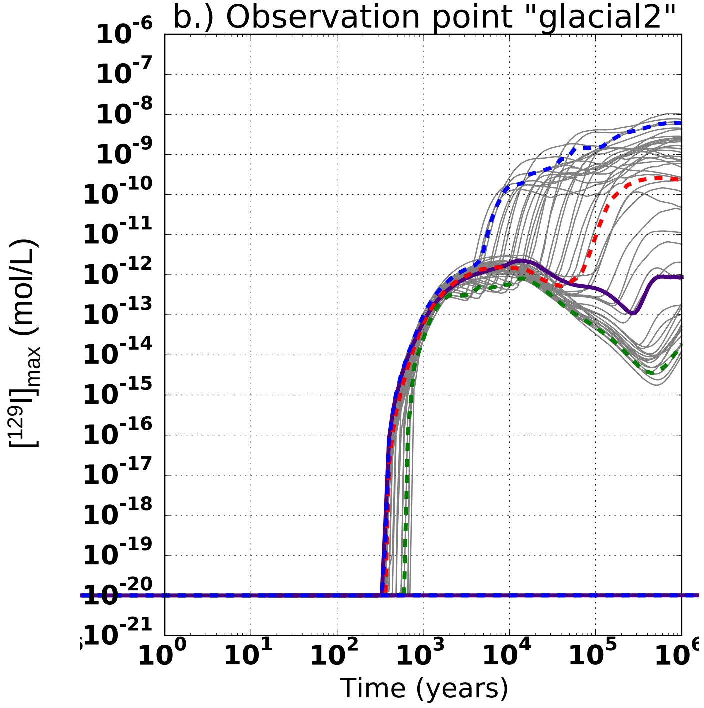
*for waste package (WP) containing 12 pressurized water reactor assemblies

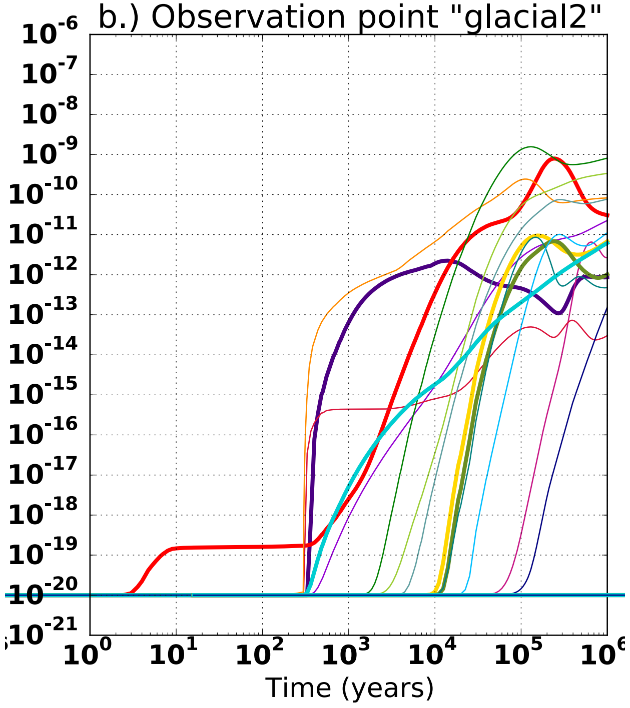


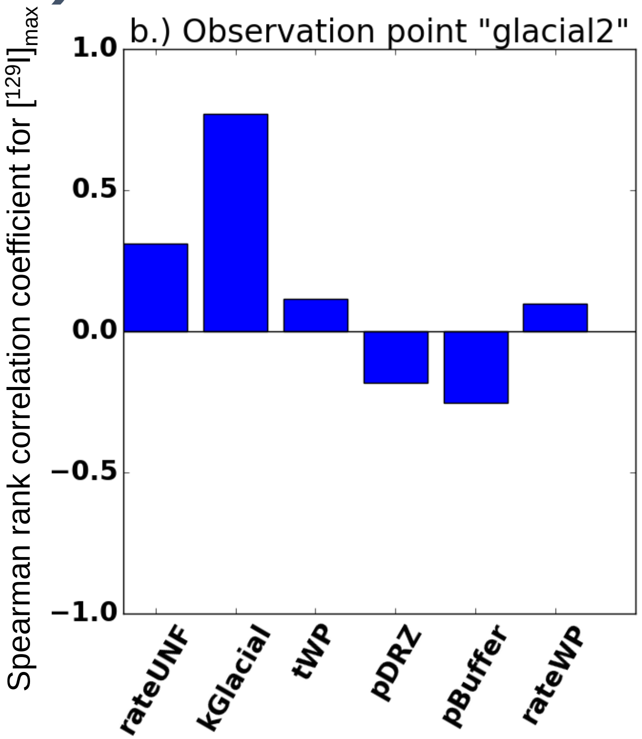
Radionuclides

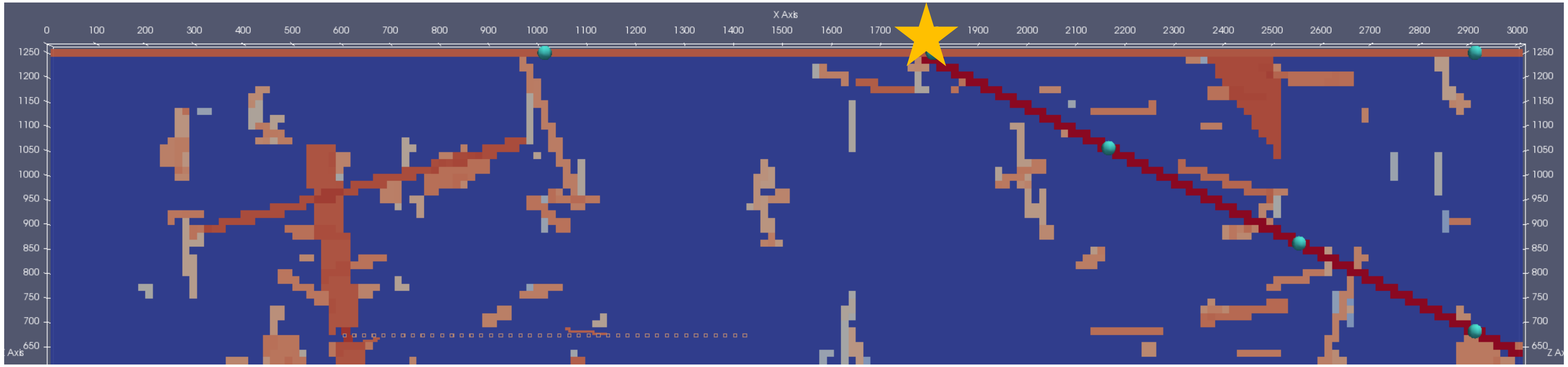
^{241}Am, ^{243}Am, ^{238}Pu, ^{240}Pu, ^{242}Pu, ^{237}Np, ^{233}U, ^{234}U, ^{236}U, ^{238}U, ^{229}Th, ^{230}Th, ^{226}Ra, ^{99}Tc, **^{129}I**, ^{135}Cs, ^{36}Cl

GDSA Outputs (for example)









Objectives and Overview of R&D Activities

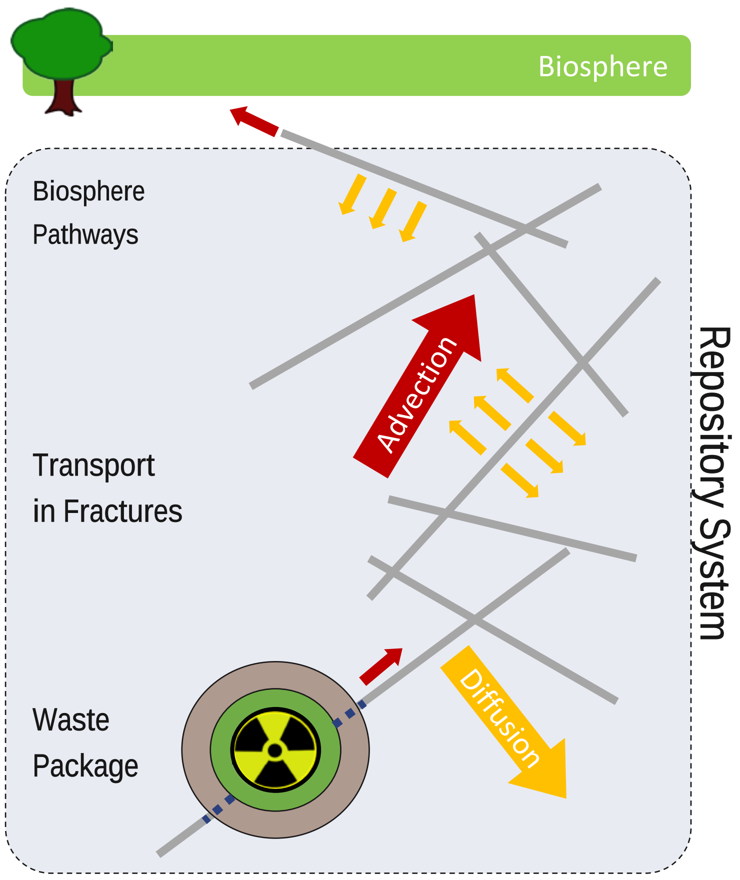
Disposal Concepts

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 at great
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; relative 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

R&D Objectives

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

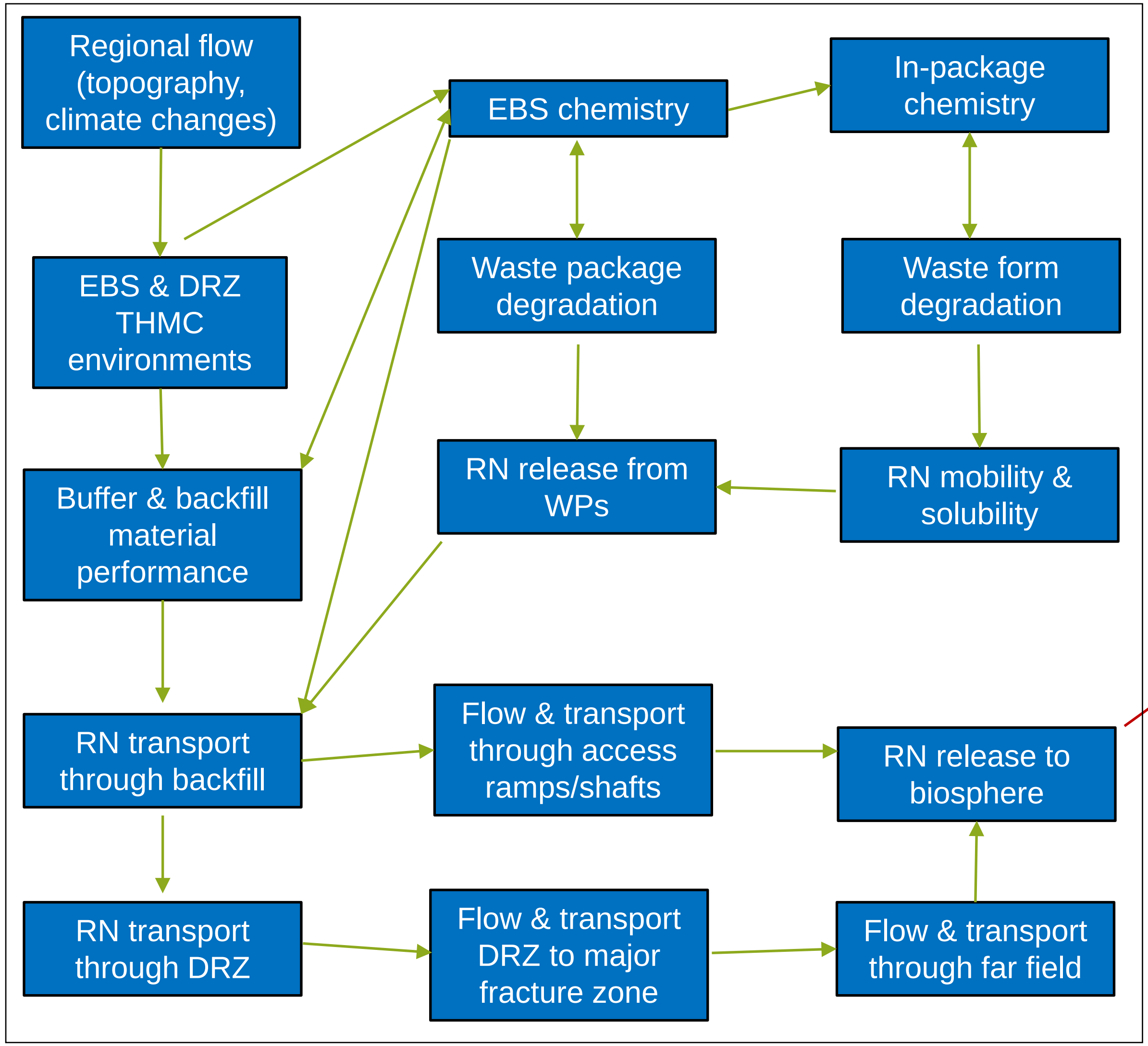
- Assist the geologic disposal safety assessment (GDSA) team to develop a robust repository performance assessment model.
- Develop basis for process modeling that enables streamlined integration with system modeling resulting in feeds to GDSA.
- Consolidate model parameter data to ensure more consistent usage.
- Understand how well the models are developed in terms of pedigree and rigor.
- Fully leverage international collaborations.
- Closely coordinate with other work packages.

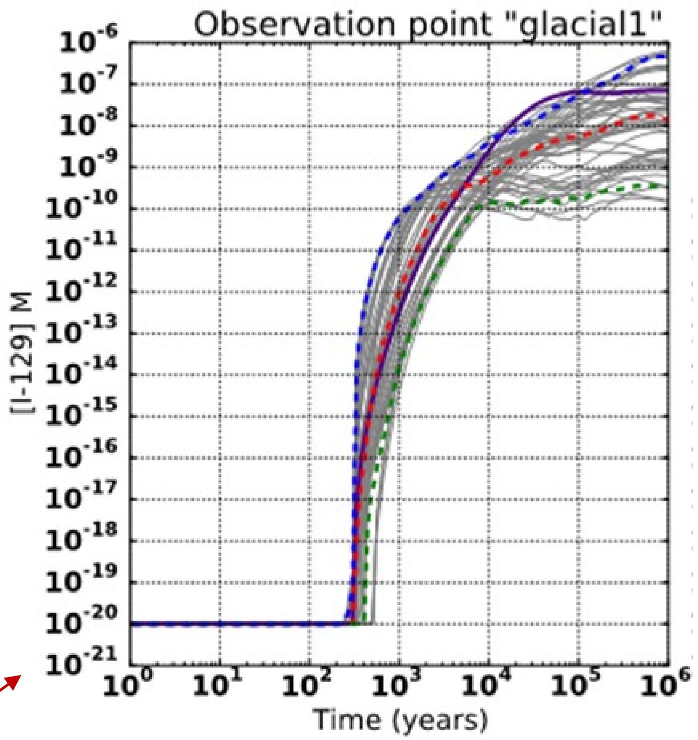


The current work focuses on: (1) better characterization and understanding of fractured media and fluid flow and transport in such media, and (2) designing effective engineered barrier systems (EBS) for waste isolation.

Key processes
- Waste form & package degradation
- Radionuclide diffusion through the EBS
- Fluid flow and transport through fracture networks in the natural barrier.

Process Model Development and Integration





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

Arrows indicate data flows between process models.

Task Status

R&D Task #	R&D Task (or Activity) Name	Accomplishments and status	Implementation in GDSA/support to process model development
C-1	**Discrete Fracture Network (DFN) Model**	• Software package dfnWorks was developed. • Workflow model for field data synthesis, tested with Mitsunami data was developed. • Significant progress was made in understanding THMC couplings in fracture networks.	• Software package dfnWorks was used to generate fracture networks for GDSA. • A simple model for the effect of stress on fracture aperture and permeability is ready for implementation.
C-2	**Flow and Transport in Fractures - modeling approaches**	• Comparison between DFN and fractured continuum models was completed. • Particle tracking vs. reactive transport was compared for uncertainty quantification. • Fluid mixing and chemical reactions in fracture networks was explored.	• Fracture continuum (or equivalent continuum) model was implemented in PFLOTRAN for far-field flow transport.
C-3	**Fracture-Matrix Diffusion**	• Matrix diffusion was incorporated in DFN mode1 and tested with data from SKB task 9. • Dual porosity model in PFLOTRAN can partly account for matrix diffusion. • FCM can also capture matrix diffusion.	• Model and data are ready for GDSA implementation.
C-4	**Lab and modeling study of EDZ - Crystalline**	• High pressure and high temperature triaxial loading system was developed. • Rigid body spring network (RBSN) model was developed for EDZ fracture evolution. • Bentonite swelling and extrusion was found to significantly reduce fracture permeability.	Experimental data are available for developing a simple model for bentonite swelling, and extrusion, and fracture plugging.
C-5	**Development of geophysical techniques for site characterization**	• Step-rate Injection Method for Fracture *In-situ* Properties (SIMFIP) was developed to measure real-time 3D mechanical deformation of rock in a borehole. • Downhole Robotic Stress Analyzer (DORSA) was developed.	The downhole test and analysis methods can be integrated into the workflow for field data analyses.
C-6	**Buffer Erosion**	• Buffer material erosion experiment was initiated. • Stabilization of buffer materials, e.g., using chemical additives, was explored. • Microfluidic cell for clay particle transport and clogging was developed.	• The conceptual Buffer Erosion Canister Corrosion (BECC) model was developed.
C-7	**Colloids in Fractures**	• Multiple site colloid transport model was developed and tested against multiple column experiments. • Pu interaction and colloid formation at clay and Fe oxide surfaces were investigated.	• Colloid-facilitated transport model and the data supporting the model are ready for GDSA implementation.
C-8	**Interaction of Buffer w/ Crystalline Rock**	• Participating in the HotBENT program. • Bentonite swelling and extrusion was found to significantly reduce fracture permeability.	• A process model for bentonite extrusion and fracture plugging yet needs to be developed.
C-9	**Development of Technical Database**	• Continued engagement with the NEA-thermodynamic database program. • Developed a geographic information system for geological data management. • Developed a model approach to using machine learning to predict thermodynamic properties of complex fluids.	• A large body of data were collected and can be used for both process model development and GDSA. • Methodology for using machine learning to develop a reduced order model for GDSA was established.
C-10	**Collate Data from International URL's**	Data have been collected from DECOVALEX, SKB, Japanese Mitsunami, South Korean KURT, and Czech URL.	The data have been used for model development and validation.
C-11	**Investigation of Fluid Flow and Transport in Low Permeability Media**	• Significant understanding has been obtained for gas migration in water-saturated compacted bentonite from the DECOVALEX program. • Demonstrated the existence of a fast advective water flow in clay interlayers. • Better understanding of non-Darcian fluid flow in clay materials was obtained.	• Basis for developing a simplified flow and transport model for GDSA is established.

To be completed

Near completion/significant progress made

Task Status (Cont.)

R&D Task #	R&D Task (or Activity) Name	Accomplishments and status	Implementation in GDSA/support to process model development
C-12	**Model Validation: Evolution of groundwater chemistry and radionuclide transport in fractured rock**	• Smart Kd approach combined with machine learning is being explored. • Radionuclide coprecipitation with secondary mineral phases is being investigated. • PFLOTRAN was updated for simulating evolving water chemistry in both the near and the field. .	• A smart Kd approach for modeling radionuclide sorption/desorption is ready for GDSA implementation.
C-13	**Evaluation and upscaling of the effects of spatial heterogeneity on radionuclide transport**	• Simulations of radionuclide transport with spatially distributed Kd values were performed, demonstrating the necessity to account for the spatial heterogeneity of Kd to appropriately capture the uncertainties of radionuclide transport and retention. • Effect of fracture network geometry on reactive transport was investigated. • Demonstrated a potential effect of heterogeneity in aperture distribution on fluid flow and transport in fracture networks.	• The approach for using spatially distributed Kd values is ready for GDSA implementation.
C-14	**Radionuclide sorption and incorporation by natural and engineered materials: Beyond a simple Kd approach**	• Iodine uptake by negatively charged clay materials through has been studied. • U transport through compacted bentonite is being investigated. • Coprecipitation of radionuclides such as Pu with corrosion products and other secondary minerals is being studied. • Long-term vs. short term sorption experiments indicate that the experimental duration affects the Kd values determined. • A relationship between sorption and coprecipitation has been explored. • Smart Kd approach using machine learning is being explored. • Sorption behavior of trivalent cations on saponite is being investigated.	• Iodine uptake data are available for incorporation into GDSA.
C-15	**Design improved backfill and seal materials**	• New additive materials to bentonite have been explored for enhanced radionuclide uptake and thermal conductivity of bentonite materials. • The transformation of smectite to illite has been studied, which demonstrates the dependence of this transformation on water/rock ratio, K concentration, and silica concentration. • Thermal effects on bentonite performance were investigated and results indicate that the thermal limit can potentially be raised from the existing assumption. • Possibility of using chemical additives to minimize buffer erosion was explored. • A capability of modeling coupled THMC processes in buffer materials was developed. • New buffer materials such as saponite for high temperature and pH has been proposed.	• Data are available for constraining realistic thermal limits for buffer materials for GDSA.
C-16	**Development of new waste package concepts and models**	• Lead or lead alloys as outer layer packaging materials were studied. • Chemical reactions at metal-bentonite interface will be investigated as a part of HotBENT tests. • High entropy alloys have been explored for waste packaging materials.	• Data are available for performance assessments of candidate package materials.

To be completed

Near completion/significant progress made

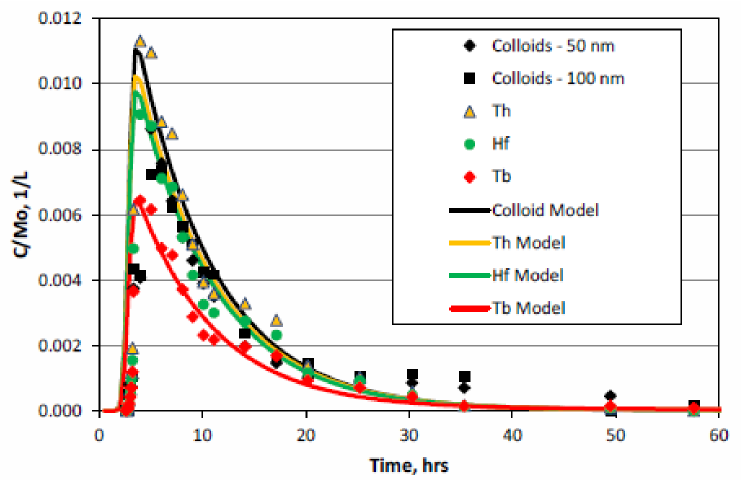
Highlights

Flow and transport in fracture networks

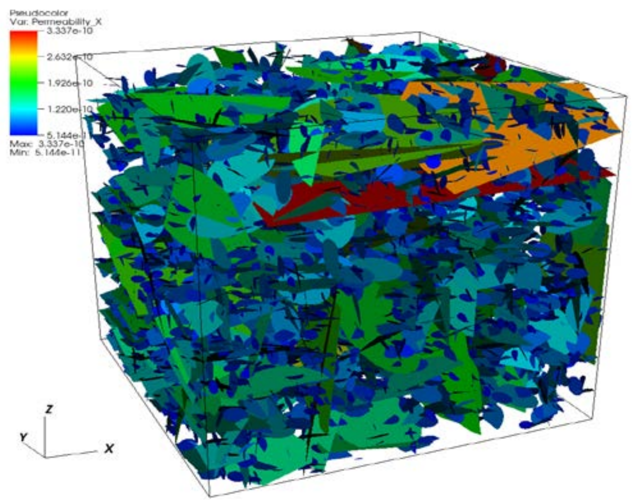
- **C-1.** Workflow for field data synthesis and fracture network representation was developed and tested with field data.
- **C-1.** Software package dfnWorks was developed and used to generate fracture networks for GDSA.
- **C-3.** Matrix diffusion was incorporated in DFN model and tested with data from SKB task 9.
- **C-7.** Colloid-facilitated transport model and the data supporting the model are ready for GDSA implementation.

Buffer materials

- **C-15.** New buffer materials such as saponite for high temperature and pH have been proposed.
- **C-8.** Bentonite swelling and extrusion was found to significantly reduce fracture permeability.
- **C-9.** Modeling approach of using machine learning to predict thermodynamic properties of chemical speciation and surface sorption was developed.
- **C-11.** Significant understanding has been obtained for fluid flow in compacted bentonite.



Column experiments and model fitting on colloid-facilitated radionuclide transport



Fracture network generated for flow and transport analyses

Summary

- **Crystalline host rock is one of the natural barrier systems studied in the Spent Fuel and Waste Disposition, Disposal Research program.**
- **Crystalline repository reference cases demonstrate safety assessment methods, drive capability development, and advance understanding of generic system behavior.**
- **Crystalline R&D integrates host rock and engineered barrier studies to advance process understanding and inform development of safety assessment capabilities.**

Questions

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