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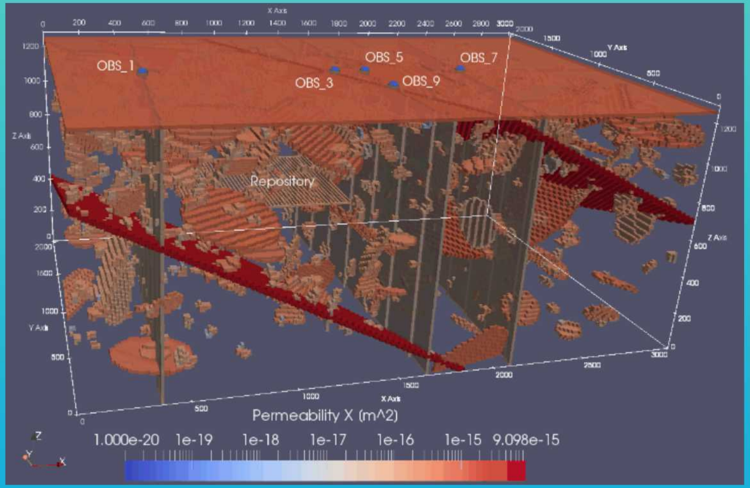

DECOVALEX-2023 Task F (Performance Assessment) Initial Specification

DECOVALEX-2023 Spring 2020 Virtual Meeting

Thursday, April 30, 2020

Lawrence Berkeley National Laboratory

Emily Stein

Sandia National Laboratories

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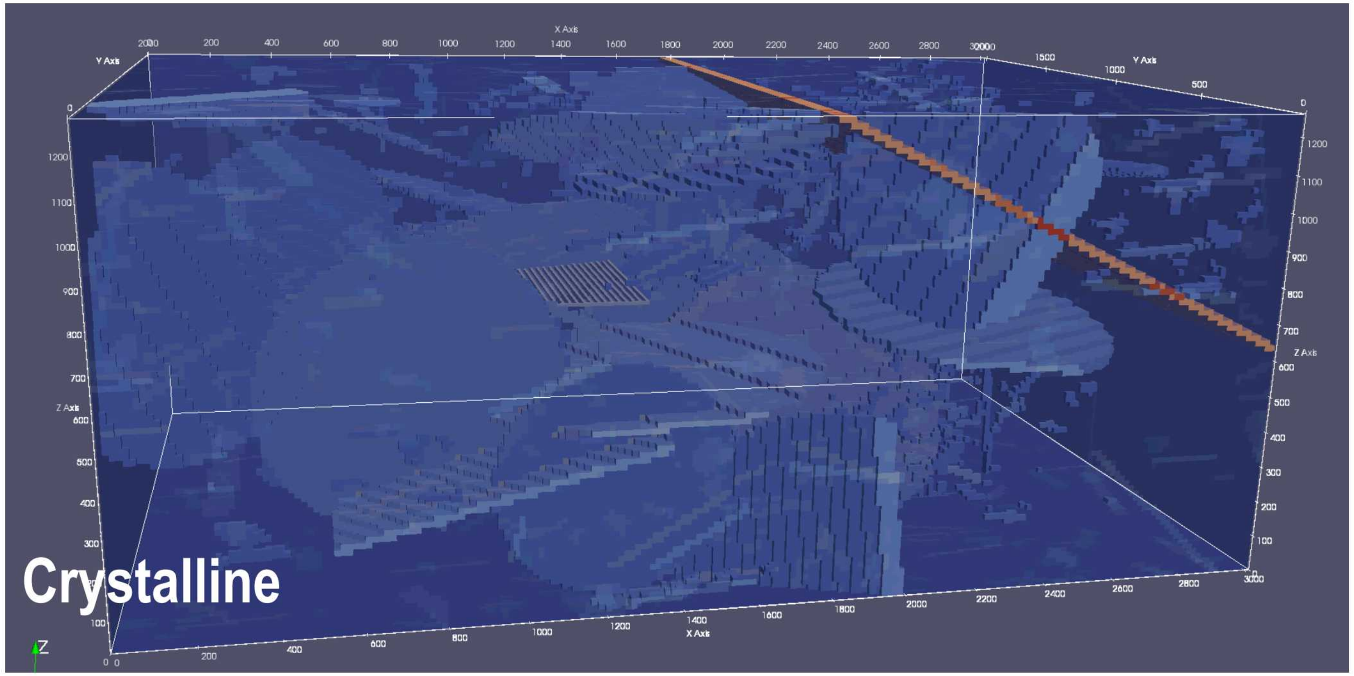
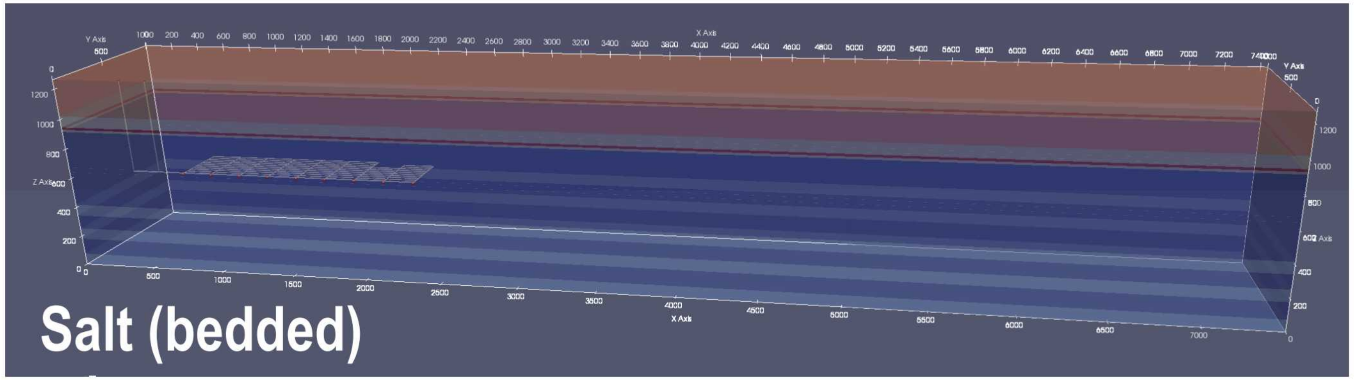
Post-closure Performance Assessment (PA)

- A tool of decision management used to
  - Quantify the repository system (post-closure) performance for all selected situations
  - Evaluate the level of confidence (taking into account identified uncertainties) in the estimated (post-closure) performance of the system
  - Provide reasonable assurance that the repository system will meet applicable (post-closure) safety standards
- Through lifetime of repository program also used iteratively to support
  - Site selection
  - Site characterization
  - Repository design
  - Data collection
  - Model development

Generic Reference Cases – Comparison of Models and Methods

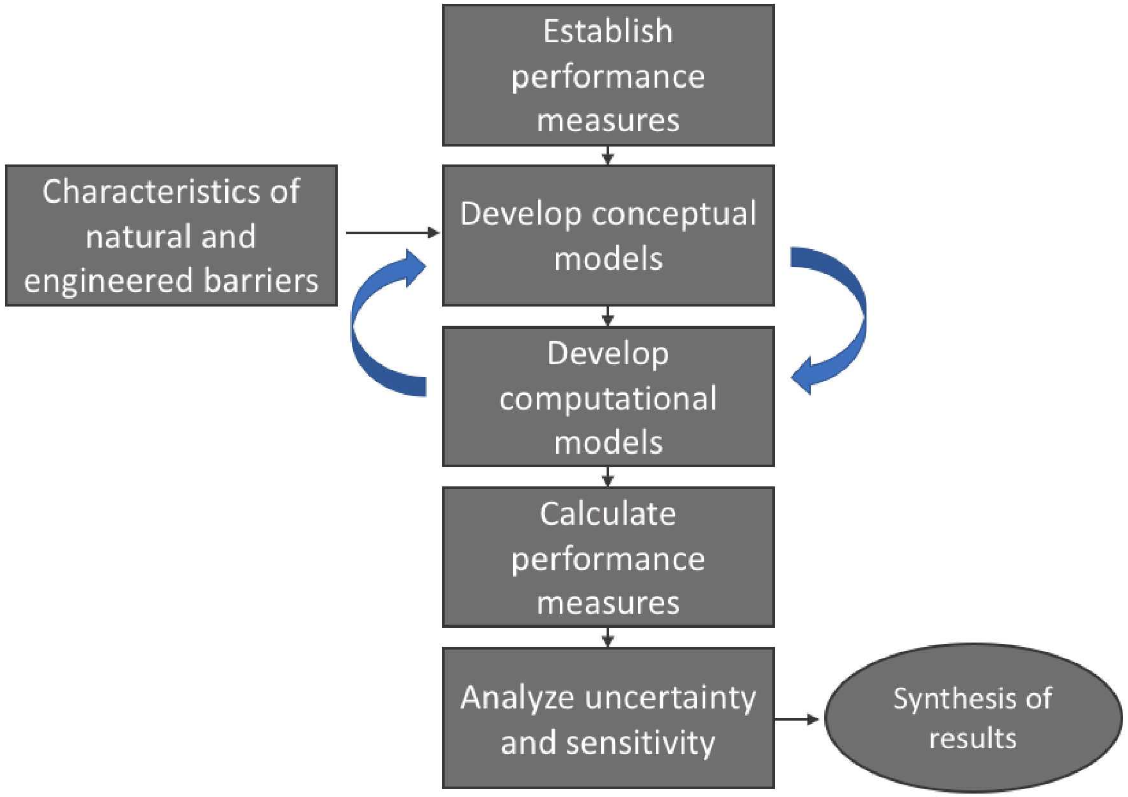




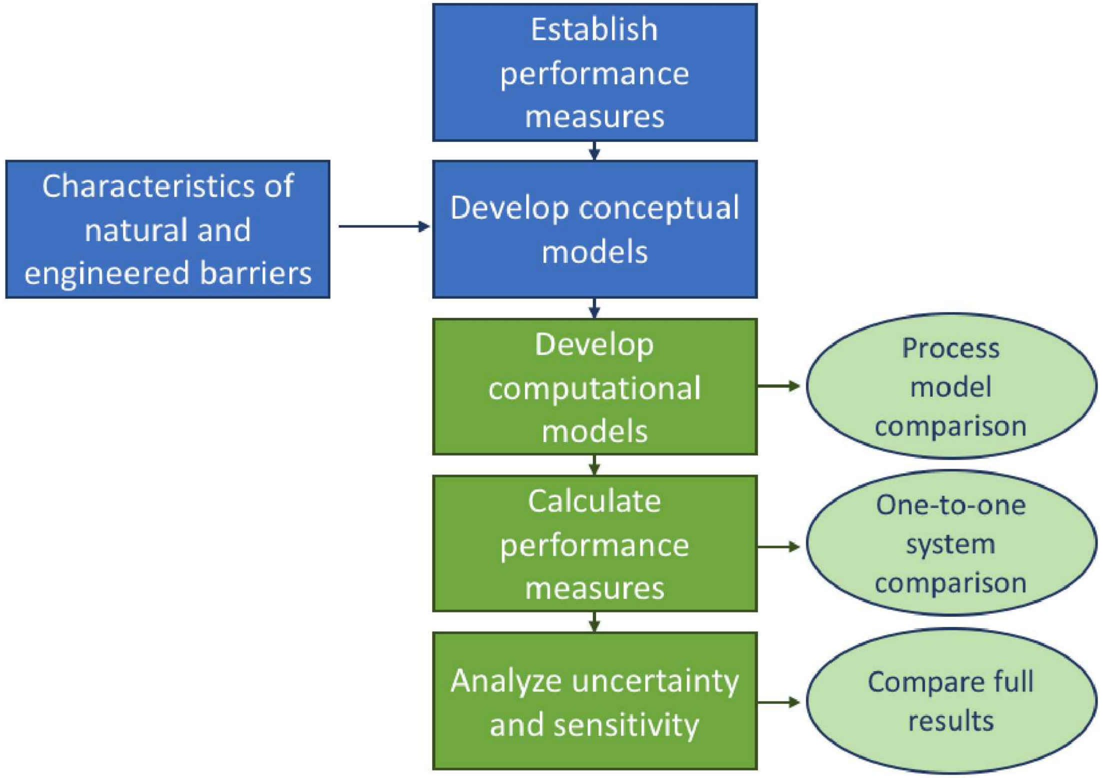
- Capability development
  - Software
  - Workflow
  - People
- Influence of modelling choices
  - Model fidelity
  - Omission/inclusion of processes
  - Coupling
- Compare to other uncertainties
  - Stochastic fracture network
  - Uncertain inputs
  - Conceptual uncertainties

Building Blocks of PA and Use in Task F

Building Blocks of PA



Task F



Task F is Atypical

Typical DECOVALEX Task

Benchmarks

↓

Test cases

↓

Blind predictions

↓

Applications

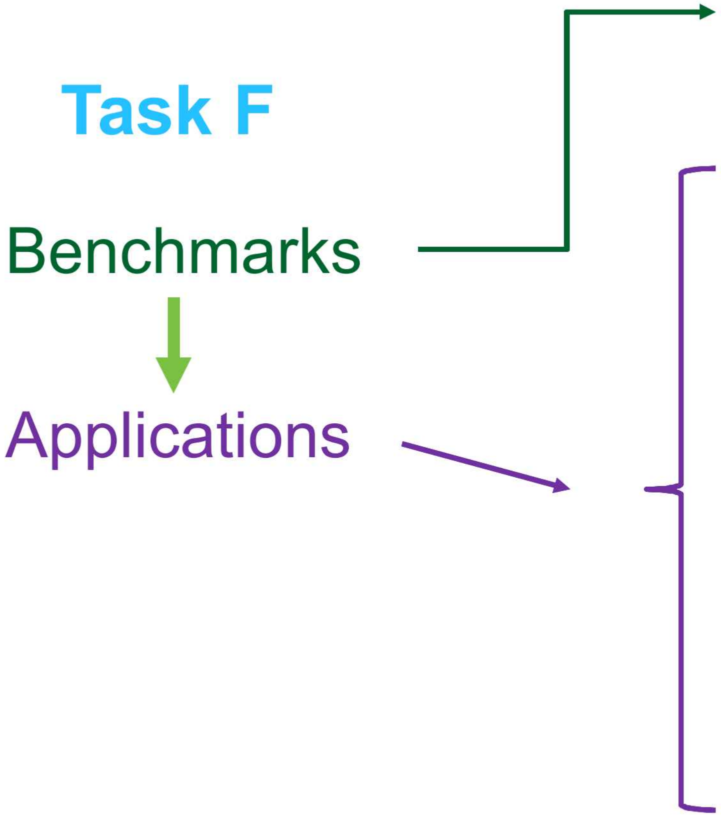
Task F

Benchmarks

↓

Applications

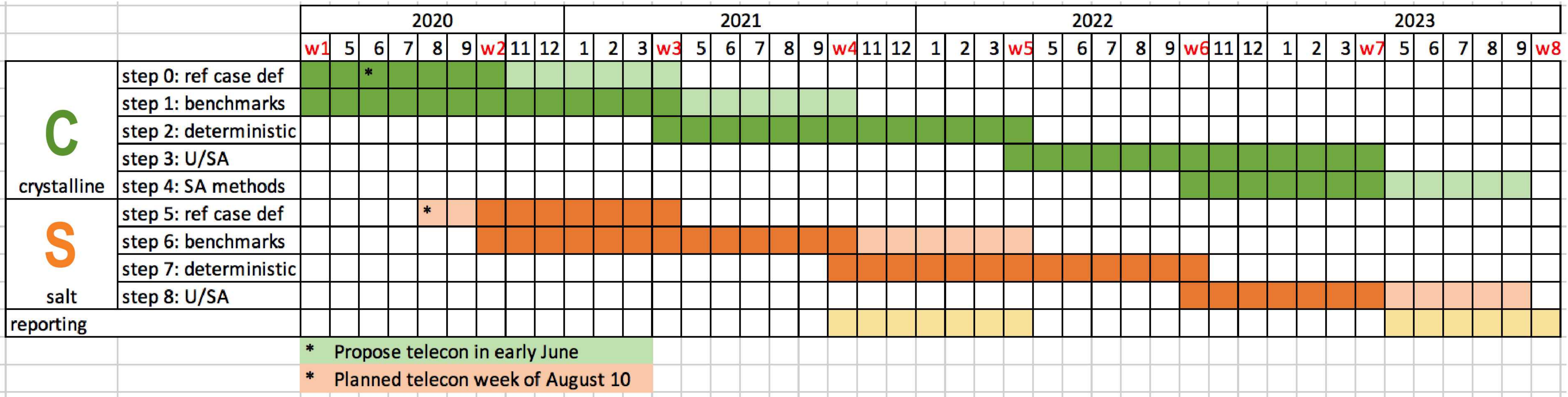
Task F Steps – Crystalline and Salt in Parallel



- Step 0 - Reference Case Definition
- Step 1 – Benchmarks/Process Models
  - Relatively simple problems that address a subset of features and/or processes
- Step 2 - Deterministic Reference Case
  - Addresses coupling between processes and results in multiple performance measures
- Step 3 - Uncertainty Propagation
  - Uncertainty in performance measures resulting from propagation of uncertainty
  - Sensitivity of performance measures to uncertain model inputs (correlation, regression)
- Step 4 - Sensitivity Analysis Methods
  - Interested teams may also compare methods of sensitivity analysis (variance decomposition, etc.)

Task F Schedule – Crystalline and Salt in Parallel

The schedule will be revised and refined as the project progresses.



Possible interfaces with other DECOVALEX-2023 Tasks

- **Task G** (Safety Implications of Fluid Flow, Shear, Thermal and Reaction Processes within Crystalline Rock Fracture Networks (SAFENET))
  - Crystalline – influence of stress state on fracture transmissivity and/or fracture slip
- **Task B** (Modelling Advection of Gas in Clays (MAGIC))
  - Crystalline – simulation of H_2 generation associated with iron corrosion and gas transport
- **Task E** (Brine Availability Test in Salt (BATS))
  - Salt – coupled processes driving brine production

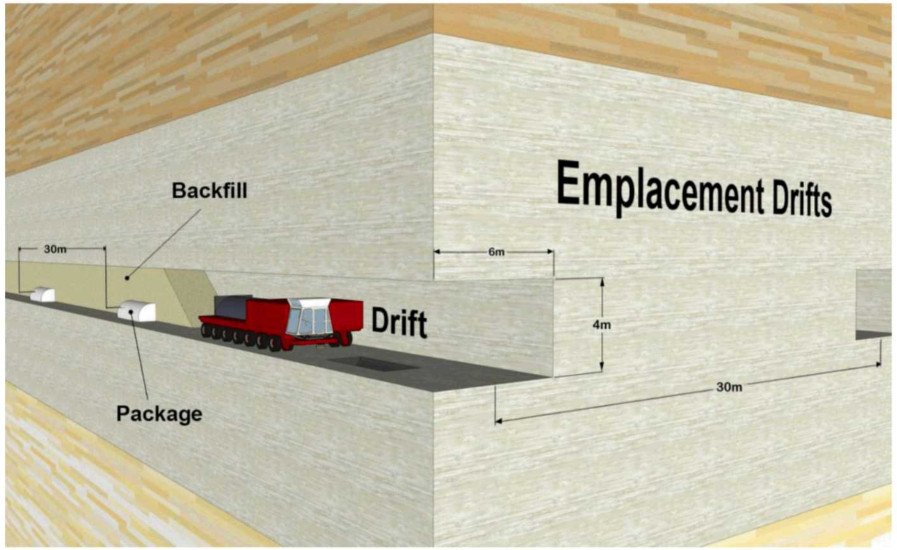
Salt Reference Case

Sources

- Reference cases developed in Germany, Netherlands, United States, other?
- New international collaboration for development of salt repository scenarios

Timing

- Lag behind crystalline ~6 months
- Telecon planned week of August 10th



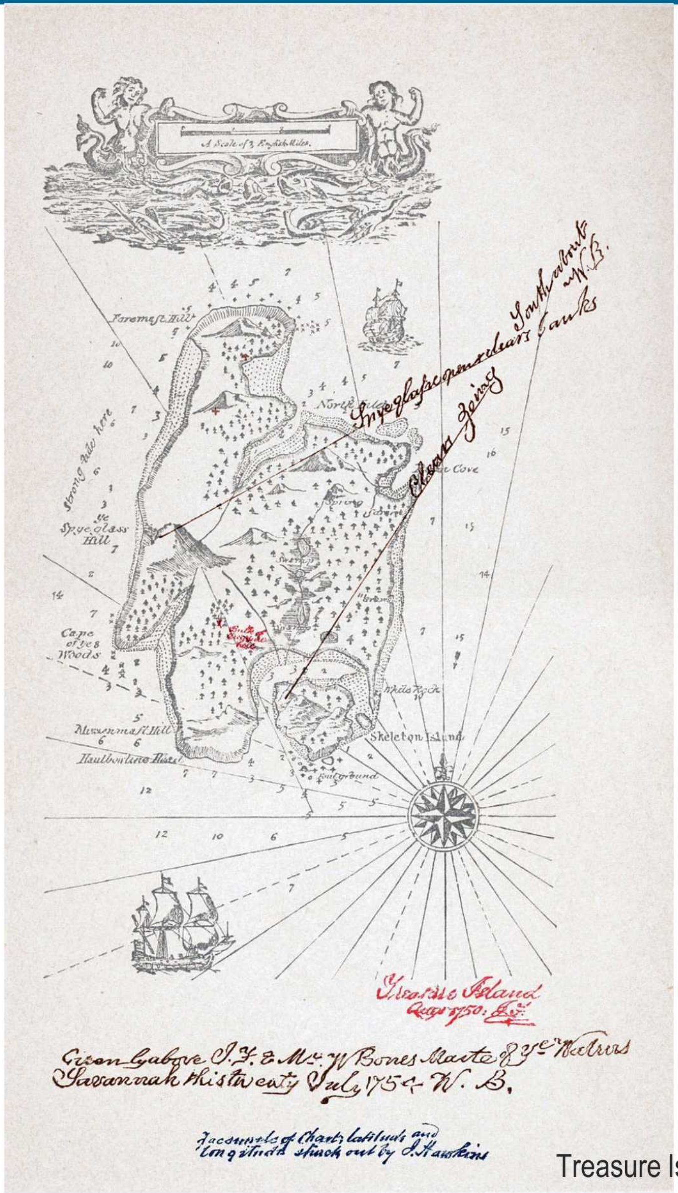
Crystalline Reference Case (Step 0)

Geologic Setting (Fictional)

- Small island
- Ground motion
- Cyclical glacial loading

Possible Canister Failure Scenarios

- Corrosion (under temperate conditions)
- Shear strain (ground motion and fracture slip)
- Either mechanism under glacial loading (fracture transmissivity as function of stress state)



Treasure Island

Emplacement Concept

KBS-3V

- 500-m deep
- Main & deposition tunnels
- Ramp and shafts
- Layout depends on
  - Thermal power
  - Large, transmissive features

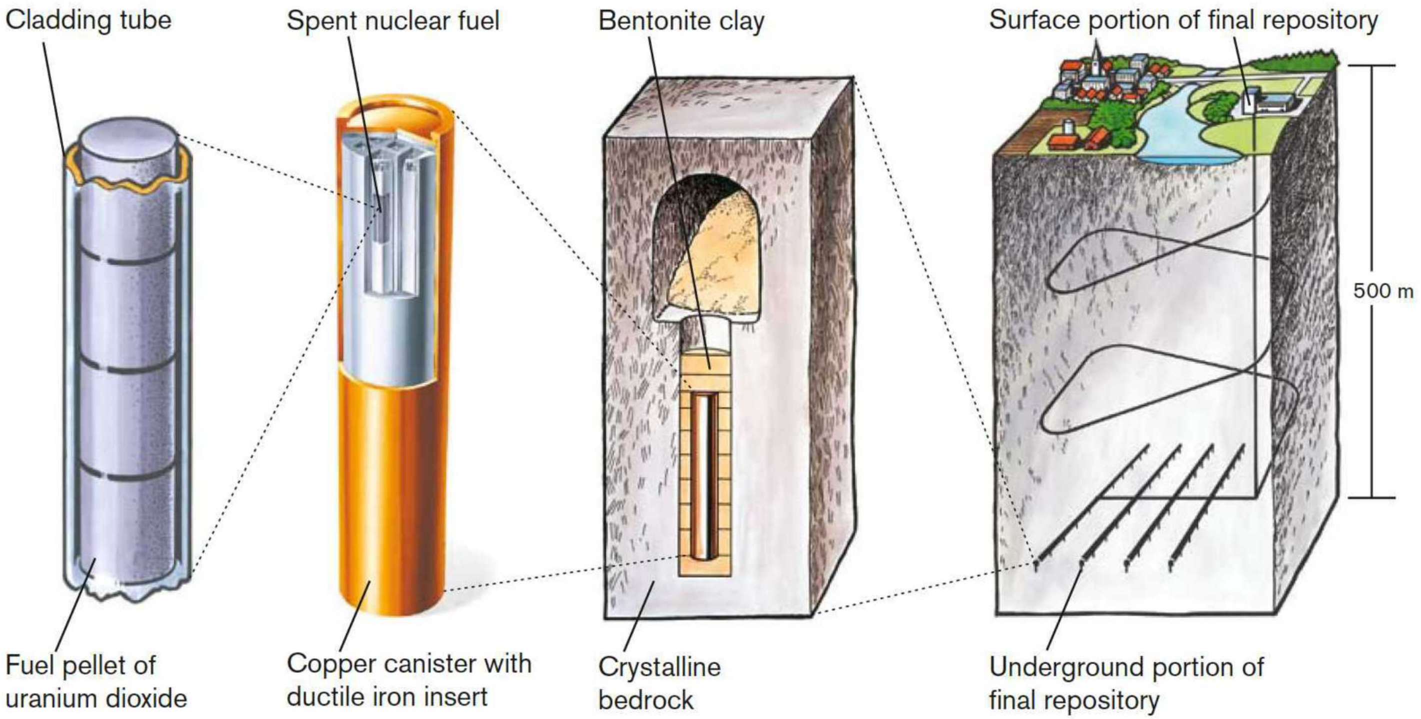


***Figure S-1.** The KBS-3 concept for disposal of spent nuclear fuel.* SKB TR-11-01

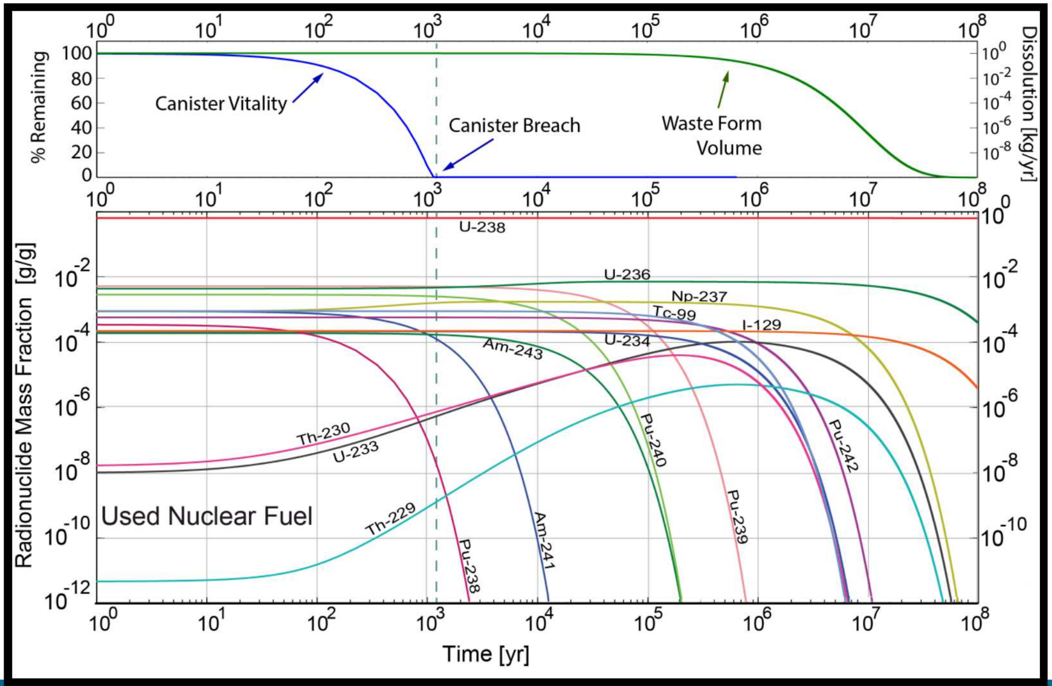
Alternatives

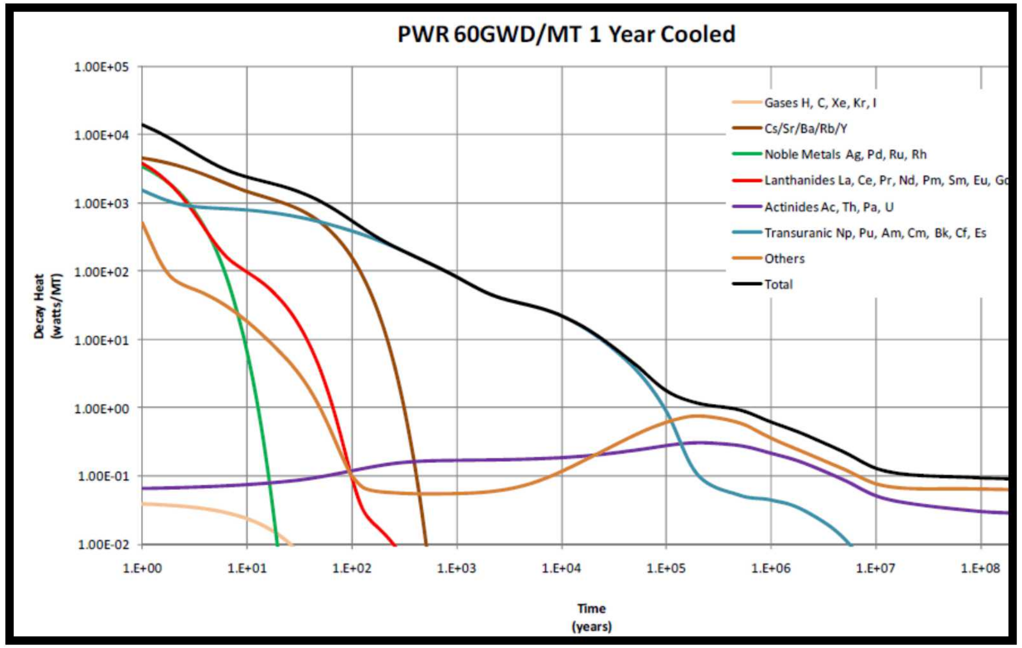
- KBS-3H
- In-drift emplacement of larger waste packages

Inventory

2500 canisters containing spent nuclear fuel (SNF)

- 4 pressurized water reactor assemblies
- 60 GW-d/MT burn-up
- 4.73 wt% ^{235}U enrichment
- 50 years out of reactor





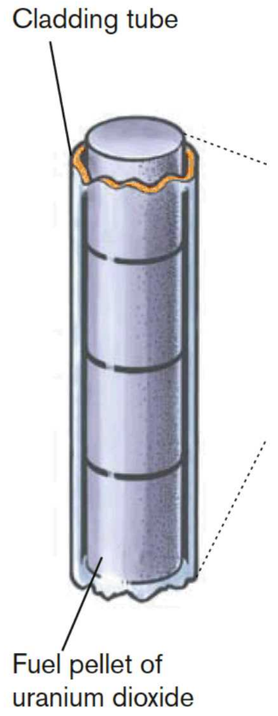
Alternatives / Additions

Lower burn-up SNF or other forms of SNF (boiling water reactor SNF, Candu SNF)

Waste Form

UO_2 SNF

- Minimum set of processes to consider
  - Radionuclide decay and ingrowth
  - Instant release of a fraction of the fission products
  - Rate-controlled dissolution of UO_2 and congruent release of radionuclides
  - Precipitation (and dissolution) of phases controlling radionuclide solubility
- Additional processes
  - Heat production
  - Radiolysis and feedback to fuel dissolution



Alternative

Teams with the capability to simulate in-canister chemistry may implement a mixed potential model for simulating the coupled electrochemical processes contributing to UO_2 dissolution.

Canister

Copper with cast iron insert

- Minimum set of processes to consider
  - Copper corrosion by reaction with HS^-
  - Shear failure due to slip on intersecting fracture
- Additional processes
  - Iron corrosion
  - Gas generation
  - Volume expansion due to corrosion products
  - Radionuclide sorption on corrosion products
  - Colloid formation

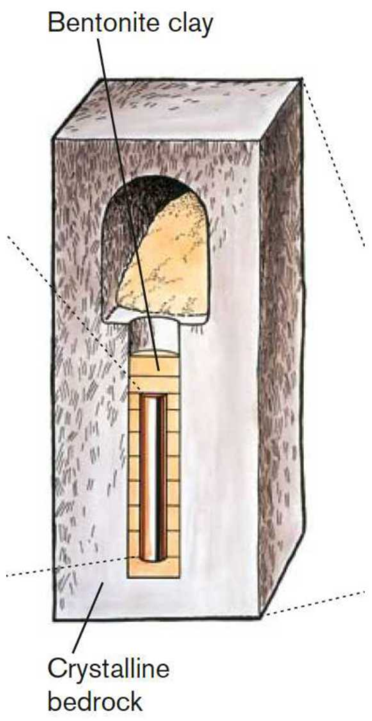
Alternative

Carbon steel outer layer with stainless steel inner layer

Buffer

Bentonite

- Minimum set of processes to consider
  - Piping/erosion
  - Diffusion, advection of corrodants
  - Diffusion, advection, decay/ingrowth of radionuclides
  - Adsorption and/or ion exchange, surface complexation
- Additional processes
  - Saturation, swelling
  - Pyrite dissolution, microbial sulfate reduction
  - Gas transport
  - Colloid formation



Alternatives

Thermal, hydraulic, mechanical, and chemical (THMC) characteristics of the bentonite buffer may be provided by a participating team or derived from SKB reports.

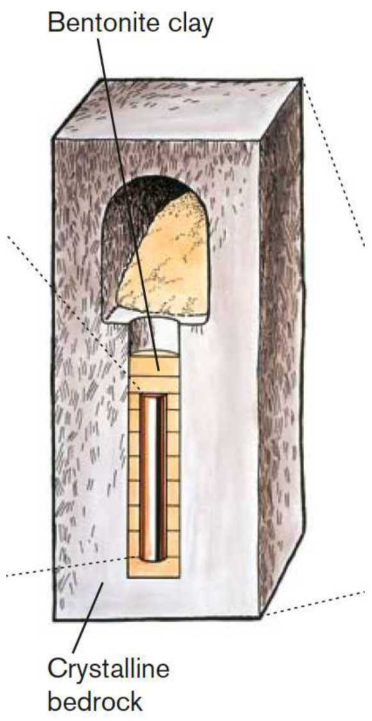
Additional Features in the Near Field

Propose to treat very simply

- Backfill (bentonite)
- Excavation damaged zone (tunnels)
- Thermal spalling (deposition holes)

Or neglect

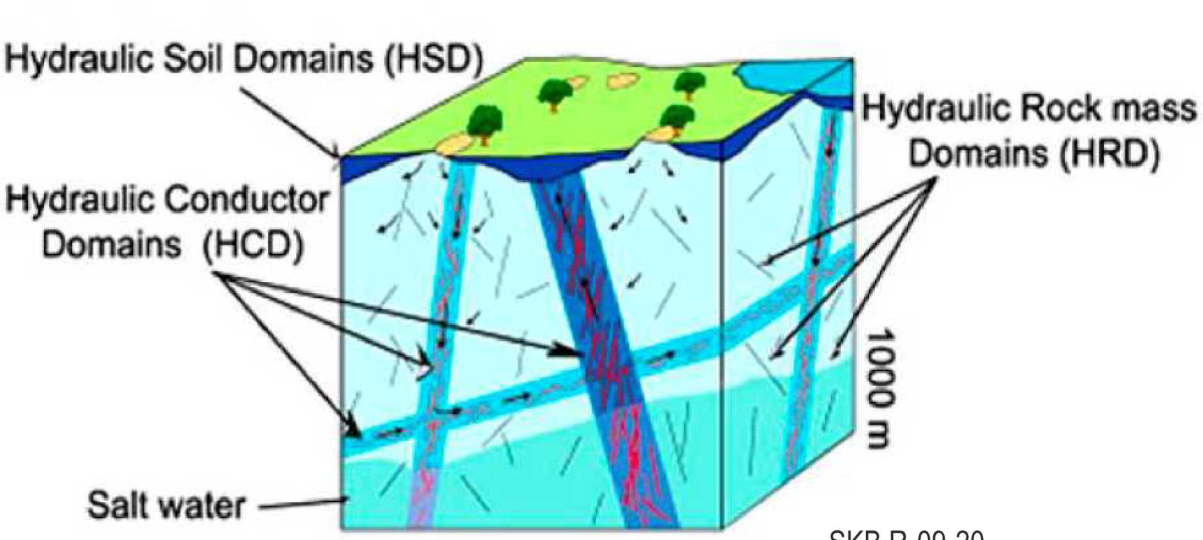
- Grout
- Drift seals
- Ramp and shafts



Fractured Host Rock

Hydraulic Conductor Domains (HCD) and Hydraulic Rock Mass Domains (HRD)

- Minimum set of processes to consider
  - Transient and/or steady flow in fractures
  - Advection, dispersion, decay/ingrowth
  - Matrix diffusion
  - Adsorption
- Additional processes
  - Slip on fractures due to changes in stress
  - Dilation and compression of fractures



SKB R-09-20

Alternatives

Fracture density and probability distributions describing size, orientation, and location of fractures in four depth zones are those of the western central hydraulic unit (CHUW) at Olkiluoto, *or*

Fracture density and probability distributions describing size, orientation, and location in three depth zones are those of HRDs FFM01/FFM06 at Forsmark.

Hydraulic Rock Mass Domains / Discrete Fracture Networks (DFNs)

Olkiluoto CHUW

- DFN parameters calibrated assuming uncorrelated, partially correlated, and correlated relationships between fracture transmissivity and size (Posiva WR-2012-42).
- Later recalibrated using a relationship expressing fracture transmissivity as a function of normal and shear stress (Posiva WR-2016-08).

Conceptual uncertainty, T = f(size)

Allows hydro-mechanical coupling

Requires more options in DFN software

Forsmark FFM01/06

- DFN parameters calibrated assuming uncorrelated, partially correlated, and correlated relationships between fracture transmissivity and size (Follin et al. 2014).
- Inherently includes only fractures that contribute to flow under the present-day stress field and cannot be used for hydromechanical coupling.

Conceptual uncertainty, T = f(size)

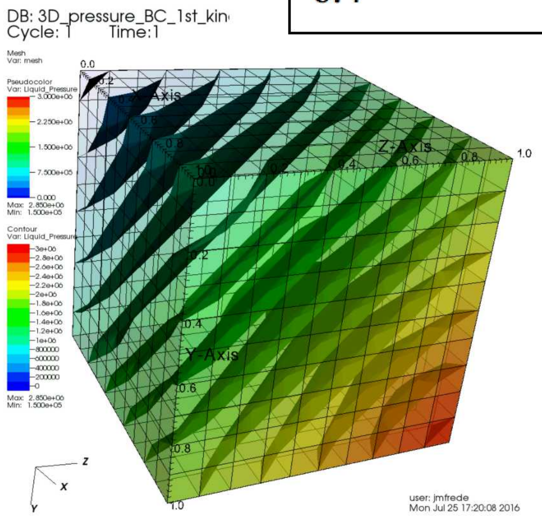
Does not allow HM coupling

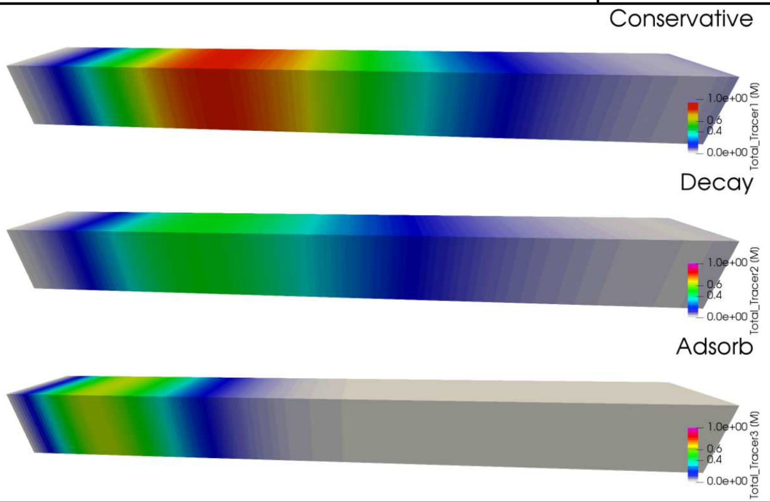
Requires fewer options in DFN software

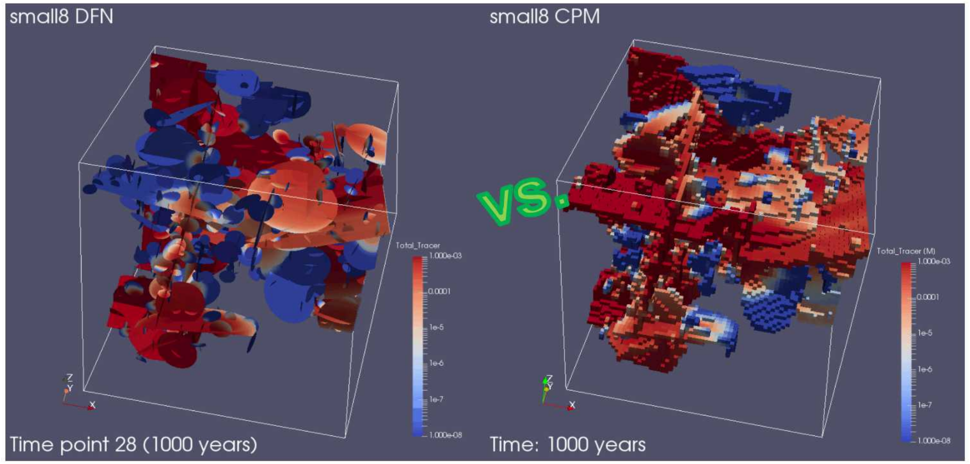
3rd Alternative DFN parameters provided by a participating team.

Crystalline Step 1 – Benchmarks and Test Cases

Section Heading	Test Cases related to:	Proposed Completion Date
6.2.1	Steady-state flow	July 2020
6.2.2	Transient advection/dispersion	July 2020
6.2.3	Matrix diffusion	November 2020
6.2.4	4-fracture network (deterministic)	November 2020
6.2.5	Stochastic fracture network	April 2021
6.3	Radionuclide source term	April 2021
6.4	Buffer and canister processes	TBD







Questions?

Thanks to DECOVALEX organizers Jens Birkholzer and Alex Bond for proposing Task F, and for their guidance in defining its boundaries.

Thanks to the members of the potential teams for early conversations about reference cases.

Thanks to Sandia National Laboratories researchers Peter Swift, Paul Mariner, Rick Jayne, Tara LaForce, Michael Nole, and Kris Kuhlman for their input to and reviews of the draft, and to Rick for compiling information for the salt reference case.

Thanks to the leadership team at the U. S. Department of Energy, Office of Nuclear Energy, Spent Fuel and Waste Science and Technology Campaign, Prasad Nair, Jorge Monroe-Rammsy, and Tim Gunter, for their support of this project.

Questions for Participants

- Team members
  - Interests
  - Experience
- Reference case
  - Crystalline
  - Salt
  - Both
- Software for
  - DFN and/or ECPM generation
  - THMC processes
  - Uncertainty and sensitivity analysis
- Computing resources