SAND2021-14107PE

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

Spent Fuel and Waste Science and Technology (SFWST)

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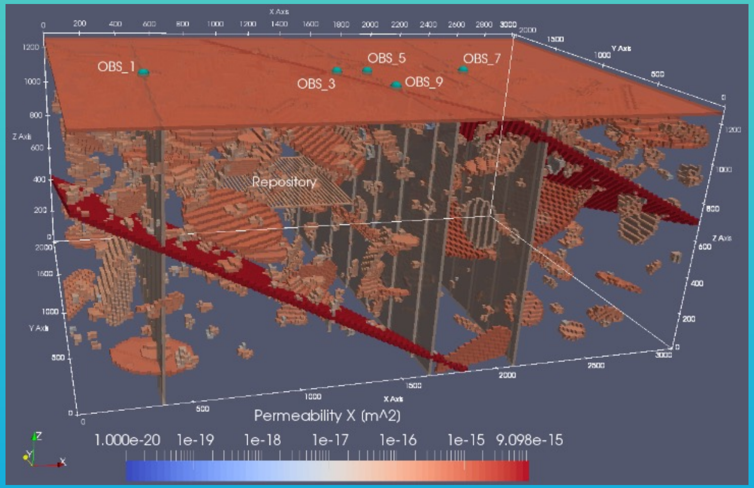


# DECOVALEX-2023 Task F (Performance Assessment) Introduction, Fall Meeting 2021

DECOVALEX-2023 Fall 2021 Meeting
Nov 8-12, 2021
Virtual Workshop

Emily Stein and Tara LaForce
Sandia National Laboratories

with thanks to Rosie Leone, Teresa Portone, and Rick Jayne

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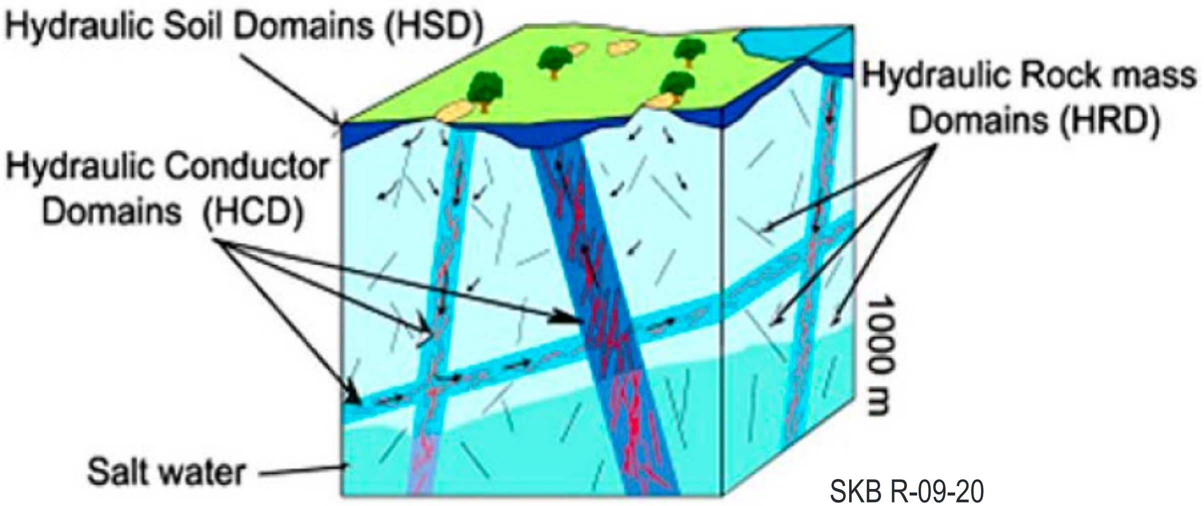
# Outline

- Task motivation and goals
- Revised task schedule
- Task F1 Crystalline
  - Where we are
  - Where we're going
  - Session agenda for Wednesday
- Task F2 Salt
  - Where we are
  - Where we're going
  - Session agenda for Tuesday

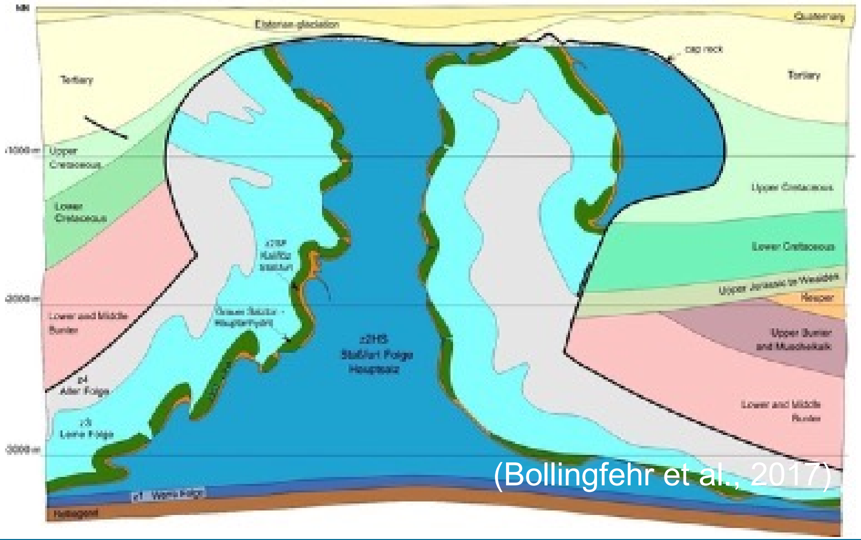
# Task Objectives – Comparison of Models and Methods

## Crystalline




SKB R-09-20

## Salt Dome

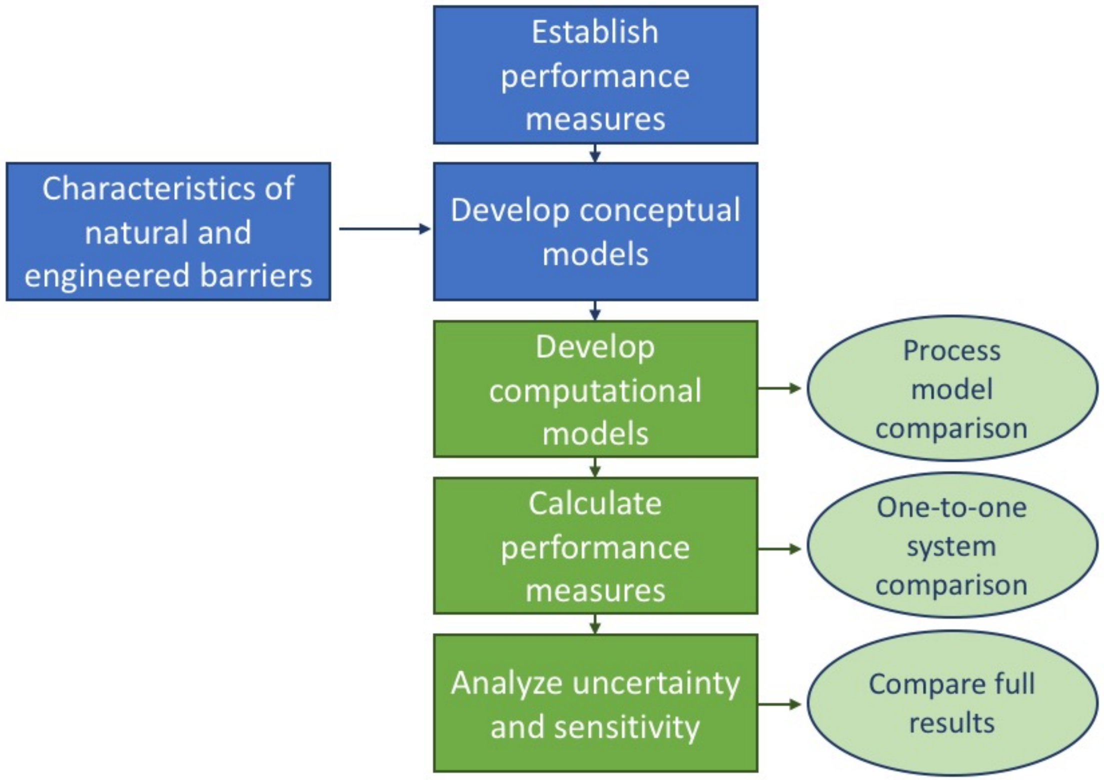


(Bollingfehr et al., 2017)

- 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
  - Scenario uncertainties

# Task Structure

- 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

## Revision 1

| | | 2020 | | | | | | | | | 2021 | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | w1 | 5 | 6 | 7 | 8 | 9 | 10 | w2 | 12 | 1 | 2 | 3 | w3 | 5 | 6 | 7 | 8 | 9 | w4 | 11 | 12 |
| C | step 0: ref case def | | | * | | * | | * | | | | | | | | | | | | | | |
| | step 1: benchmarks | | | | | | | | X | | | * | * | X | | | | | | | | |
| | step 2: deterministic | | | | | | | | | | | | | X | | | | | | | | |
| | step 3: U/SA | | | | | | | | | | | | | | | | | | | | | |
| crystalline | step 4: SA methods | | | | | | | | | | | | | | | | | | | | | |
| S | step 0: ref case def | | | | | * | * | | X | | * | * | * | X | | | | | | | | |
| | step 1: benchmarks | | | | | | | | | | | | | | | | | | | | | |
| | step 2: deterministic | | | | | | | | | | | | | X | | | | | | | | |
| | step 3: U/SA | | | | | | | | | | | | | | | | | | | | | |
| salt | step 4: SA methods | | | | | | | | | | | | | | | | | | | | | |
| reporting | | | | | | | | | | | | | | | | | | | | | | |

| | | 2022 | | | | | | | | | | | | 2023 | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 1 | 2 | 3 | w5 | 5 | 6 | 7 | 8 | 9 | w6 | 11 | 12 | 1 | 2 | 3 | w7 | 5 | 6 | 7 | 8 | 9 | w8 |
| C | step 0: ref case def | | | | | | | | | | | | | | | | | | | | | | |
| | step 1: benchmarks | | | | | | | | | | | | | | | | | | | | | | |
| | step 2: deterministic | | | | | | | | | | | | | | | | | | | | | | |
| | step 3: U/SA | | | | | | | | | | | | | | | | | | | | | | |
| crystalline | step 4: SA methods | | | | | | | | | | | | | | | | | | | | | | |
| S | step 0: ref case def | | | | | | | | | | | | | | | | | | | | | | |
| | step 1: benchmarks | | | | | | | | | | | | | | | | | | | | | | |
| | step 2: deterministic | | | | | | | | | | | | | | | | | | | | | | |
| | step 3: U/SA | | | | | | | | | | | | | | | | | | | | | | |
| salt | step 4: SA methods | | | | | | | | | | | | | | | | | | | | | | |
| reporting | | | | | | | | | | | | | | | | | | | | | | | |

* Virtual task meetings

X DECOVALEX Workshops

## Revision 2

| | | 2020 | | | | | | | | | 2021 | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | w1 | 5 | 6 | 7 | 8 | 9 | 10 | w2 | 12 | 1 | 2 | 3 | w3 | 5 | 6 | 7 | 8 | 9 | 10 | w4 | 12 |
| C | step 0: ref case def | | | * | | * | | * | X | | | * | * | X | | * | | * | | | X | |
| | step 1: benchmarks | | | | | | | | | | | | | | | | | | | | | |
| | step 2: deterministic | | | | | | | | | | | | | | | | | | | | | |
| | step 3: U/SA | | | | | | | | | | | | | | | | | | | | | |
| crystalline | step 4: SA methods | | | | | | | | | | | | | | | | | | | | | |
| S | step 0: ref case def | | | | | * | * | | X | | * | * | * | X | | | * | | * | * | | |
| | step 1: benchmarks | | | | | | | | | | | | | | | | | | | | | |
| | step 2: deterministic | | | | | | | | | | | | | | | | | | | | X | |
| | step 3: U/SA | | | | | | | | | | | | | | | | | | | | | |
| salt | step 4: SA methods | | | | | | | | | | | | | | | | | | | | | |
| reporting | | | | | | | | | | | | | | | | | | | | | | |

| | | 2022 | | | | | | | | | | | | 2023 | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 1 | 2 | 3 | w5 | 5 | 6 | 7 | 8 | 9 | w6 | 11 | 12 | 1 | 2 | 3 | w7 | 5 | 6 | 7 | 8 | 9 | w8 |
| C | step 0: ref case def | | | | | | | | | | | | | | | | | | | | | | |
| | step 1: benchmarks | | | | | | | | | | | | | | | | | | | | | | |
| | step 2: deterministic | | | | | | | | | | | | | | | | | | | | | | |
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| | step 1: benchmarks | | | | | | | | | | | | | | | | | | | | | | |
| | step 2: deterministic | | | | | | | | | | | | | | | | | | | | | | |
| | step 3: U/SA | | | | | | | | | | | | | | | | | | | | | | |
| salt | step 4: SA methods | | | | | | | | | | | | | | | | | | | | | | |
| reporting | | | | | | | | | | | | | | | | | | | | | | | |

* Virtual task meetings

X DECOVALEX Workshops

# Crystalline

Task F1

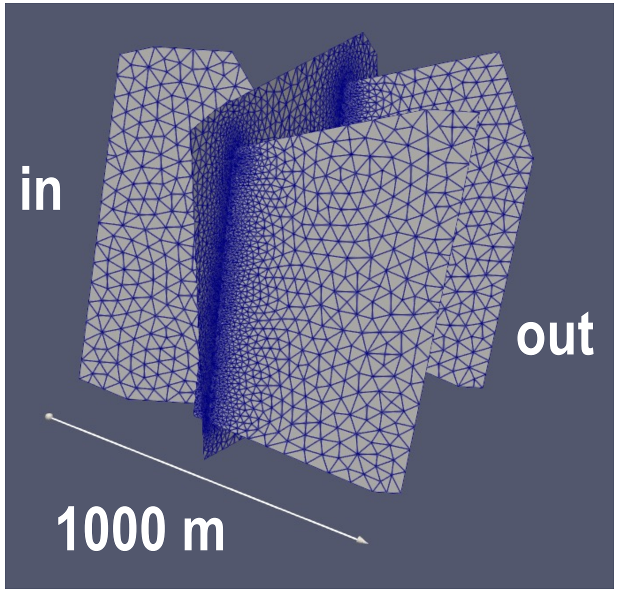
Wednesday, 10 Nov

0500-0900 (PST)

# Crystalline Benchmarks and Test Cases

| Test Cases |
| --- |
| Steady-state flow |
| Transient advection/dispersion |
| Matrix diffusion |
| 4-fracture network (deterministic) |
| Stochastic fracture network |
| Radionuclide source term |
| Buffer and canister processes |

# 4-Fracture Network




Discrete Fracture Network (DFN)

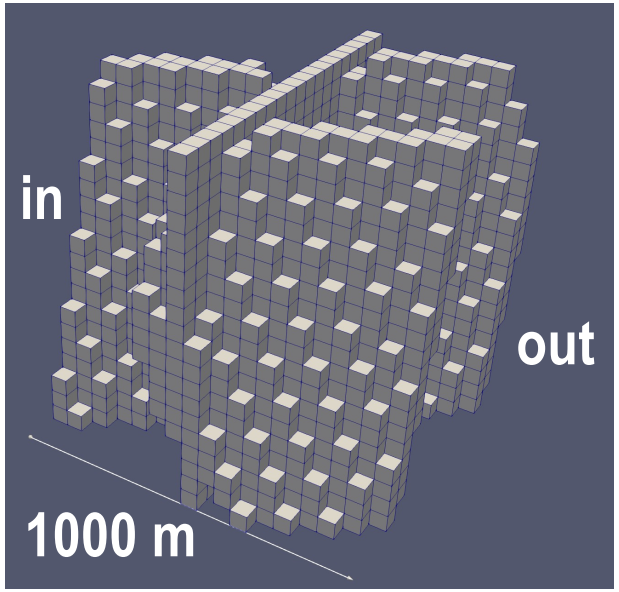
or

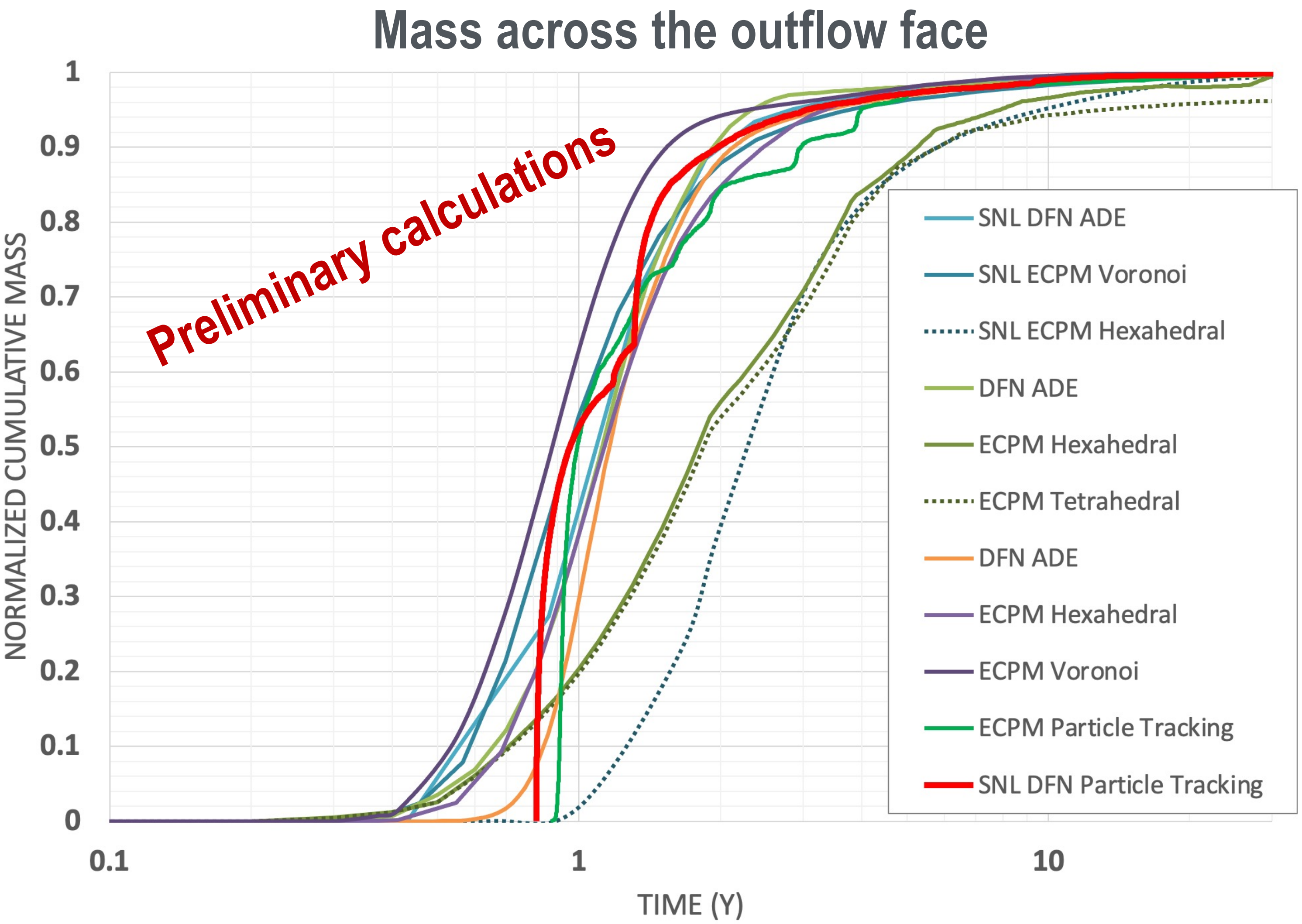
Equivalent Continuous Porous Medium (ECPM)

Particle Tracking

or

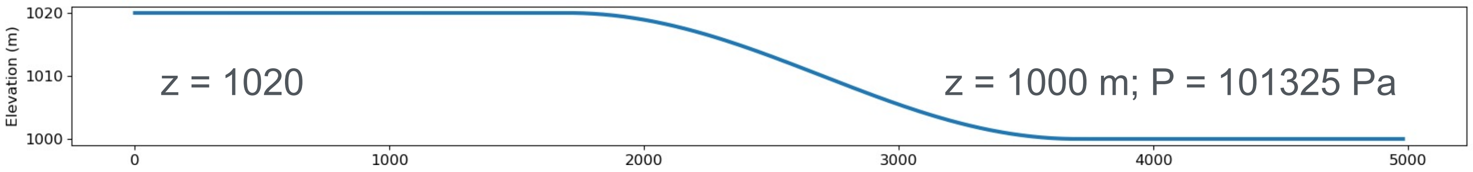
Advection-Dispersion Equation

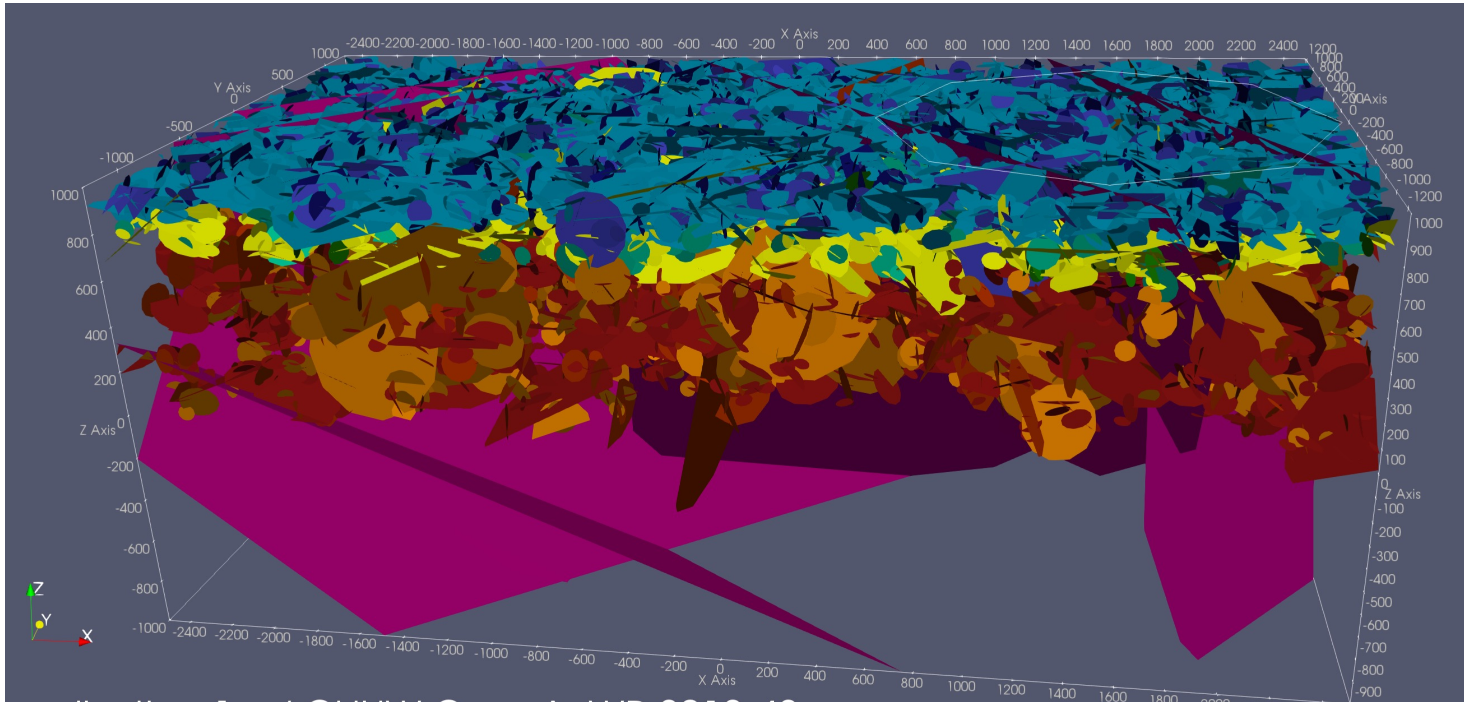


# Crystalline Reference Case – Natural Barrier System

- Loosely based on Olkiluoto
  - Deterministic fracture zones based on Brittle Fracture Zones (WR-2017-32)
  - Stochastic discrete fracture network based on Central Hydraulic Unit West (WR-2012-42)
    - 3 depth zones each with 3 fracture sets
  - Can relate fracture transmissivity to normal and shear stress (WR-2016-08)




realization 1 w/ CHUW Case A; WR 2012-42

# Crystalline Reference Case – Engineered Barrier System

- KBS-3V emplacement concept
  - Spent nuclear fuel
  - Copper canister
  - Cast iron insert
  - Bentonite buffer in boreholes
  - Bentonite backfill in drifts
  - 2500 canisters

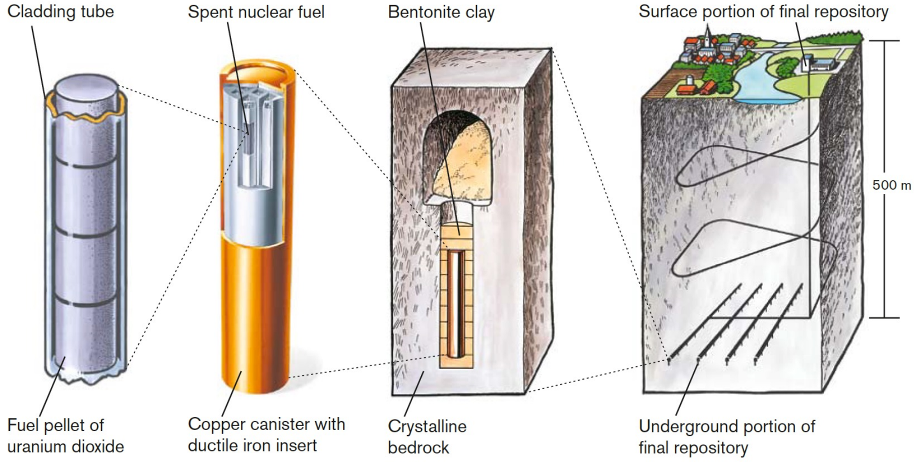



*Figure S-1. The KBS-3 concept for disposal of spent nuclear fuel.*

- Conservative tracer transport
  - Similar to instant release and slow release of $^{129}I$

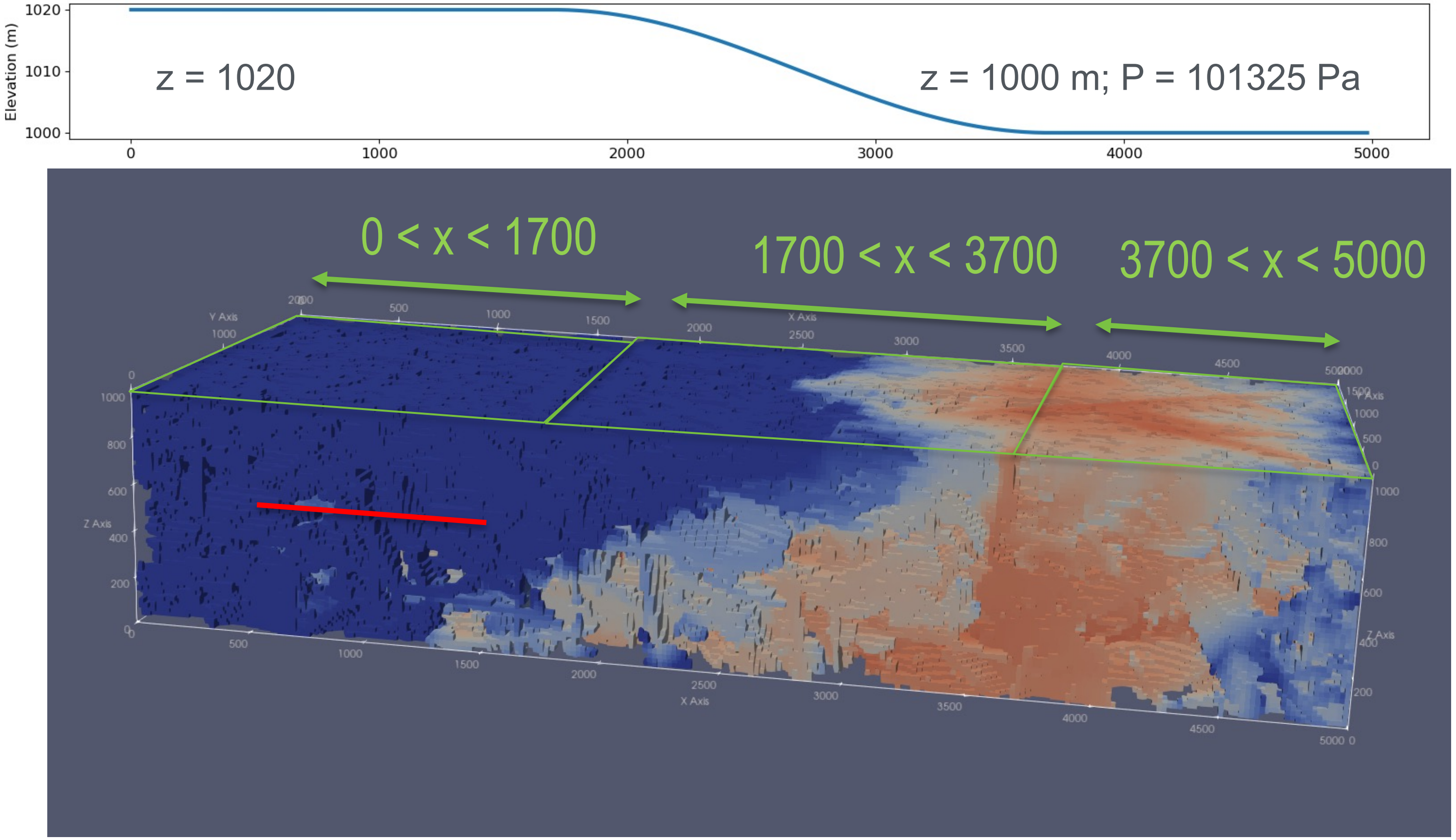
| | Atomic weight | Inventory per waste package | Release mechanism |
|---|---|---|---|
| Tracer 1 | 128.9 g/mol | 0.545 g | Instant |
| Tracer 2 | 128.9 g/mol | 4.9 g | $10^{-7}$/year |

**Initial simulations –**

**Tracer transport in steady state flow field**

# Outputs for Comparison

- Function of time
  - Total tracer mass flow across top surface where x > 3700 m
  - Maximum tracer mass flow across top surface where 1700 < x < 3700
  - Mass tracer remaining in the repository
- Steady state
  - Total liquid flow across top surface where x < 1700, etc.



# Task F1, Crystalline: Day 3, Stream 1 (Wednesday)

| Start | Finish | Duration | Topic | Speaker |
|---|---|---|---|---|
| 5:00 | 5:10 | 10 | Welcome | Emily Stein |
| 5:10 | 5:30 | 20 | Structural Geology - Look ahead | Carlo Dietl |
| **Presentations re '4frac' and '4frac+ revised' benchmarks:** | | | | |
| 5:30 | 5:45 | 15 | DOE | Rosie Leone |
| 5:45 | 6:00 | 15 | KAERI | Jaewon Lee and Jung-Woo Kim |
| 6:00 | 6:15 | 15 | INER/Taipower | Chieh-Chun Chang |
| 6:15 | 6:30 | 15 | SURAO | Marek Vencl and Ondrej Miklas |
| 6:30 | 6:40 | 10 | Discussion - what remains to be done? | All |
| 6:40 | 6:50 | 10 | Break | |
| **Presentations re reference case:** | | | | |
| 6:50 | 7:00 | 10 | Reference Case Overview | Emily Stein |
| 7:00 | 7:10 | 10 | Calculating effective permeability | Teresa Portone |
| 7:10 | 7:20 | 10 | Discussion - what constraints should be provided to teams? | All |
| **Presentations re modeling approach:** | | | | |
| 7:20 | 7:35 | 15 | DOE | Rosie Leone |
| 7:35 | 7:50 | 15 | KAERI | Jaewon Lee and Jung-Woo Kim |
| 7:50 | 8:05 | 15 | INER/Taipower | Chieh-Chun Chang |
| 8:05 | 8:20 | 15 | CNSC | Son Nguyen |
| 8:20 | 8:35 | 15 | BGR | Jan Thiedau |
| 8:35 | 8:50 | 15 | Discussion - what tweaks to do we need to make? | |
| 8:50 | 9:00 | 10 | Wrap-Up | Emily Stein |

# Salt

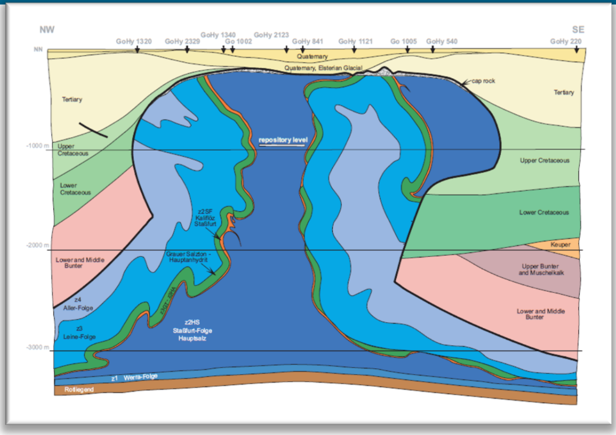
Task F2

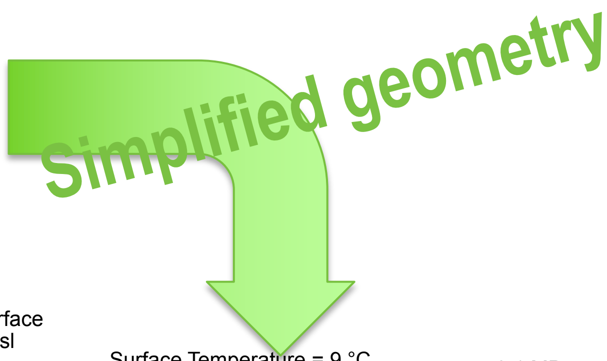
Tuesday, 9 Nov

0600-0900 (PST)

# Salt Reference Case – Natural Barrier System

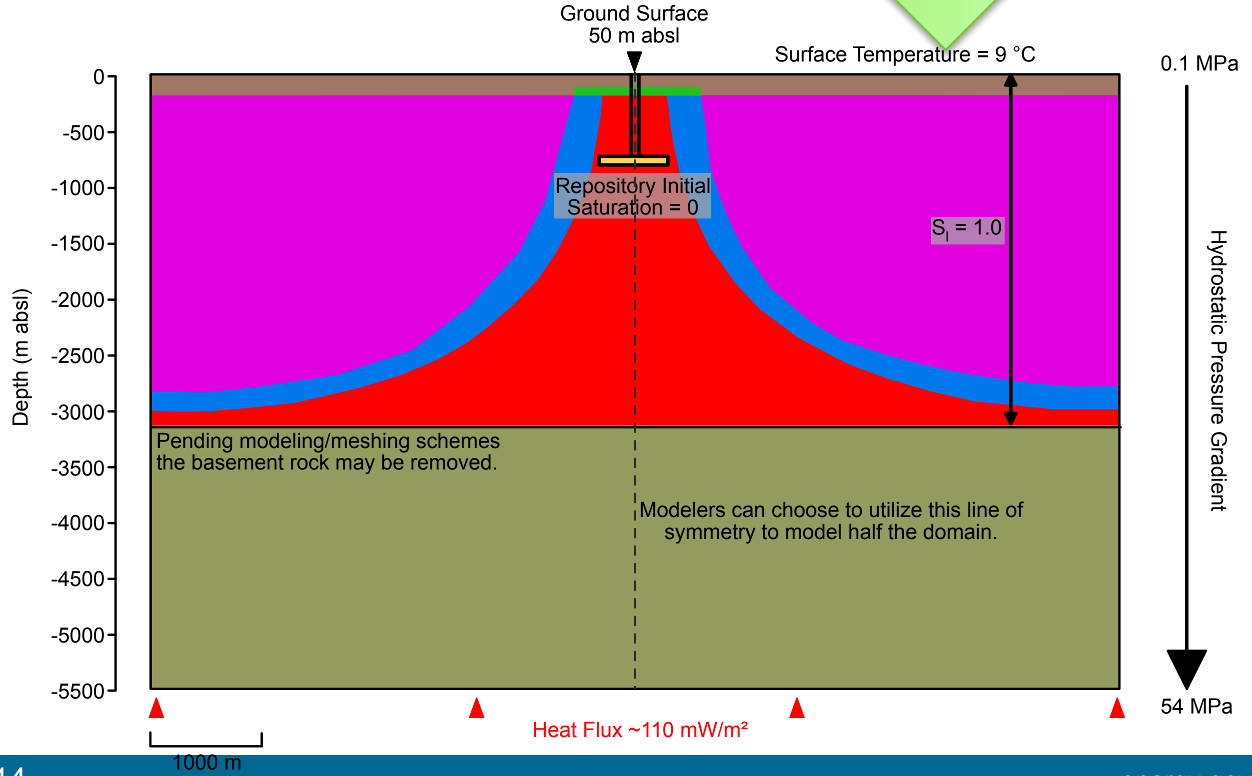
- Salt dome
  - No flowing groundwater ($\sim 0.1$ vol-% brine)
  - Openings creep closed ($> 10^0 - 10^2$ yr )
  - Crushed salt heals to intact salt






| | Intrinsic Permeability (m²) | Porosity | Thermal Conductivity (W/m²) [a] |
|---|---|---|---|
| **Overburden** | 1.00E-15 | 0.2 | 2.3 |
| **Caprock** | 1.00E-18 | 0.4 | 2.2 |
| **Basin Fill** | 1.00E-17 | 0.25 | 2.5 |
| **Anhydrite/Potash** | 1.00E-19 | 0.05 | 2.6 |
| **Domal Salt** | 1.00E-22[a] | 0.001 [a] | 5.5 |
| **Basement** | 1.00E-21 [a] | 0.01 | 2.7 |

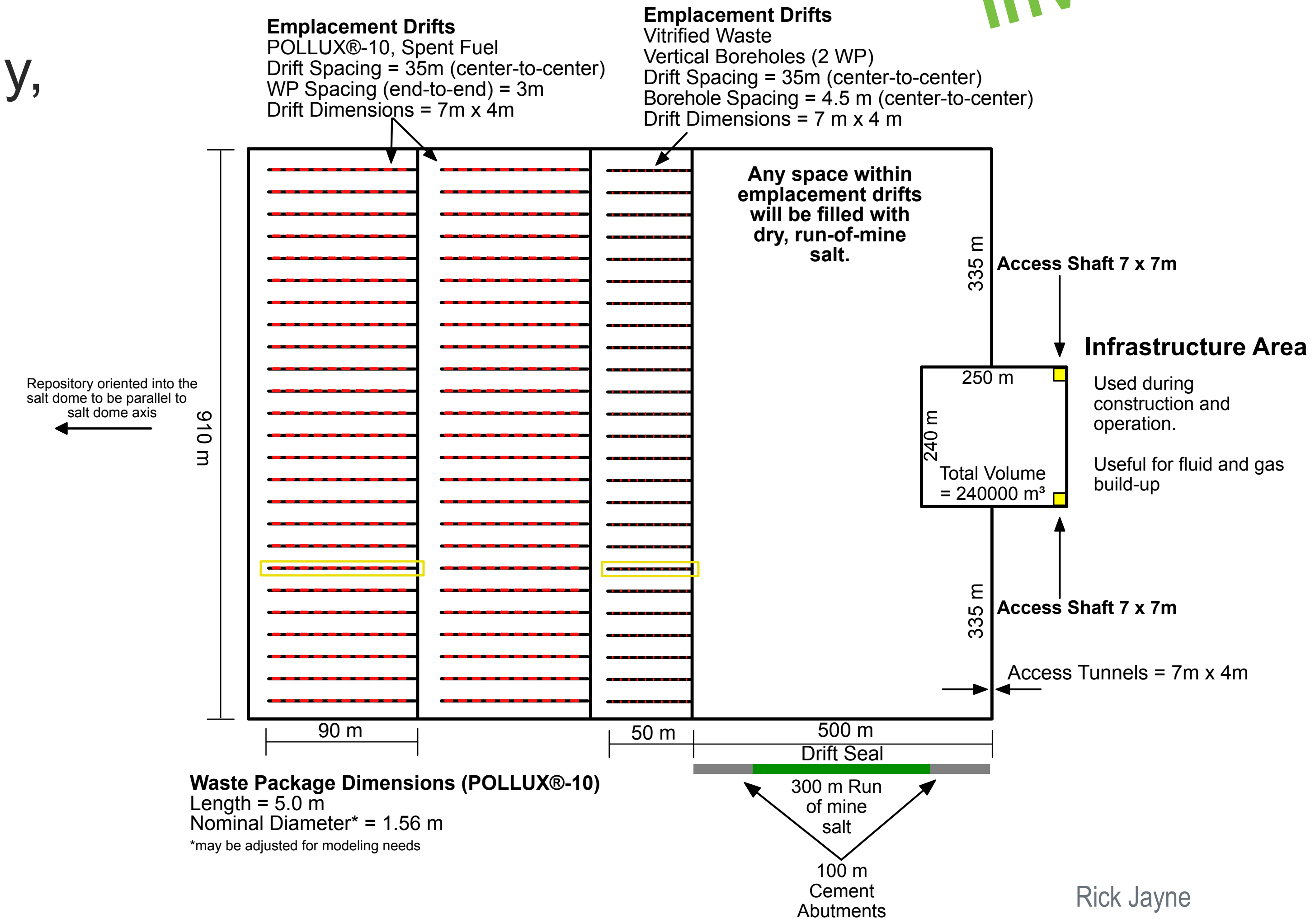
**[a] from Bertrams et al., 2020**
**All other parameters taken from general geologic property tables.**



# Salt Reference Case – Engineered Barrier System

Small inventory

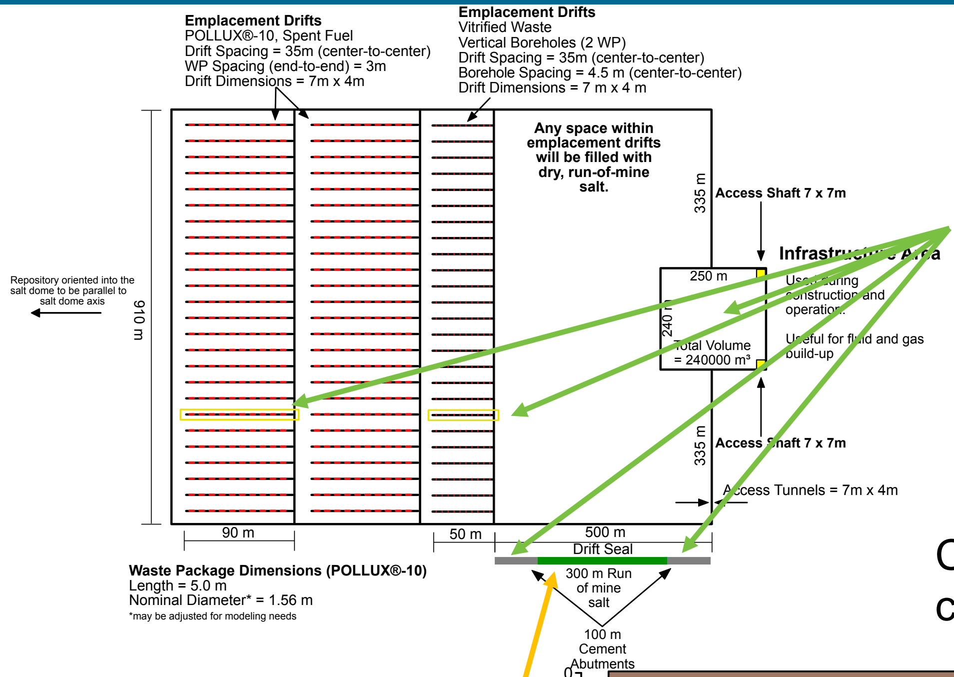
- Features borrowed from Germany, Netherlands, United States
  - Glass waste form (25 drifts of 10)
    - Borehole in floor placement
  - Spent nuclear fuel (50 drifts of 10)
    - In-drift placement
  - Crushed salt backfill in drifts
  - Gravel in infrastructure area
  - Concrete drift seals (2)
  - Layered shaft seals (2)




Rick Jayne

# Model Development and Comparison

- Disturbed scenario: shaft seals fail at 1000 y
  - Bulk permeability increases from $5\times10^{-17}m^2$ to $5\times10^{-15}m^2$
- Staged model development
  1. Flow + radionuclide transport
  2. + multiphase flow
  3. + drift convergence
  4. + heat flow and temperature-dependence of drift convergence
  5. + model uncertainty in backfill consolidation model
  6. (+ gas generation)



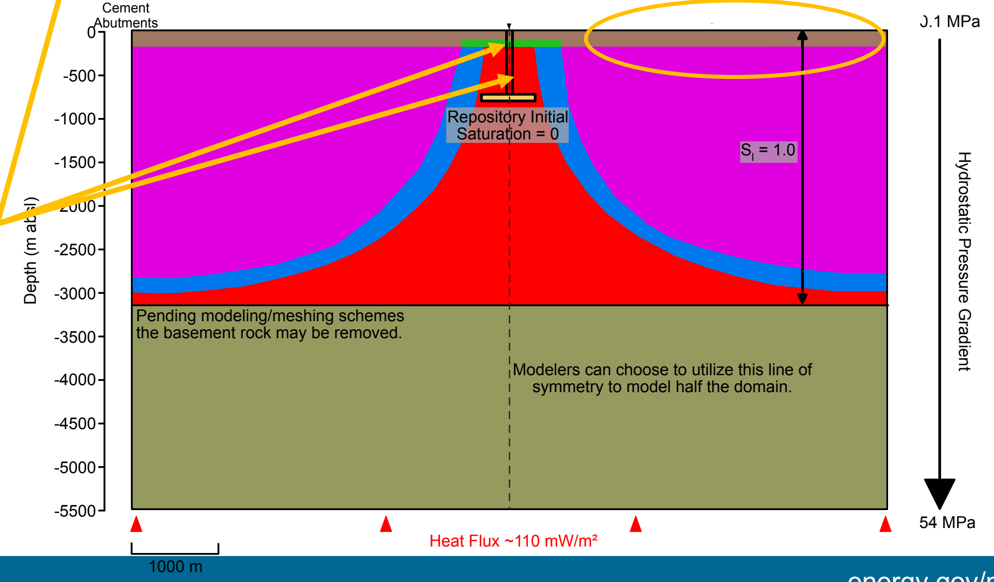

Compare:
- Saturation
- Pressure
- Radionuclide mass

vs time

Compare:
- Liquid flux
- Radionuclide flux

vs time

Compare radionuclide concentration vs time



# Task F2, Salt: Day 2, Stream 2 (Tuesday 0600 to 0900 PST)

**Welcome & Review of benchmarks (30 min)**
DOE – Tara LaForce

**Modeling Approaches to Perfomance Assessment Case (120 min)**

a. COVRA – Jeroen Bartol
b. GRS – Tanja Frank
c. Quintessa – Steve Benbow and Alex Bond
d. DOE – Rick Jayne

*10 min break*

**Discussion (20 min)**
•Plan for interim reporting
•Plan virtual meetings

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