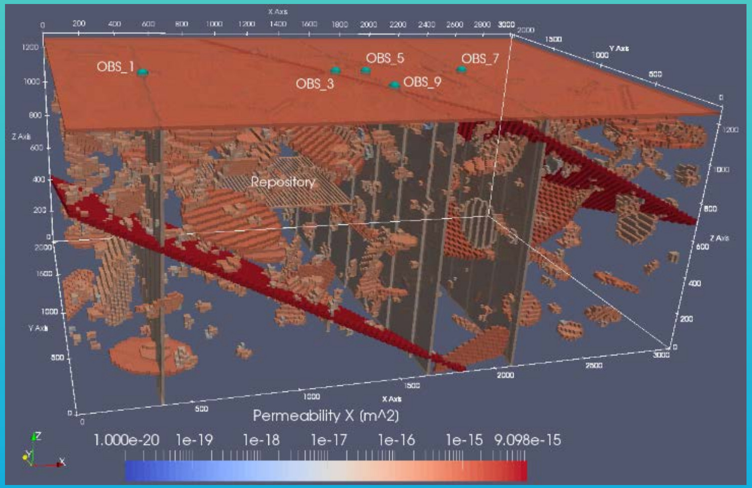
U.S. DEPARTMENT OF ENERGY | Office of NUCLEAR ENERGY

Spent Fuel and Waste Science and Technology (SFWST)

Clean. Reliable. Nuclear.



DECOVALEX Task F: Case Study in Integrating Insight and Experience from the International Community in GDSA

U. S. Nuclear Waste Technical Review Board
Fall Workshop
November 3-4, 2021

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Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

NNSA

SAND2021-13708 PE

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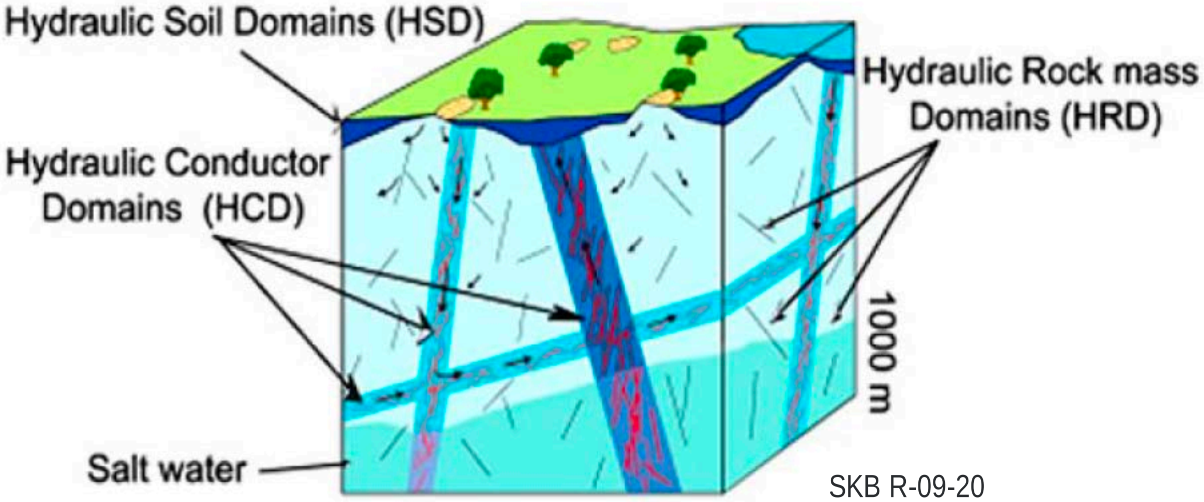
Outline

- DECOVALEX (Development of COupled models and their VALidation against Experiments) Task F Structure
- Crystalline Benchmarks
- Crystalline Reference Case
- Salt Reference Case

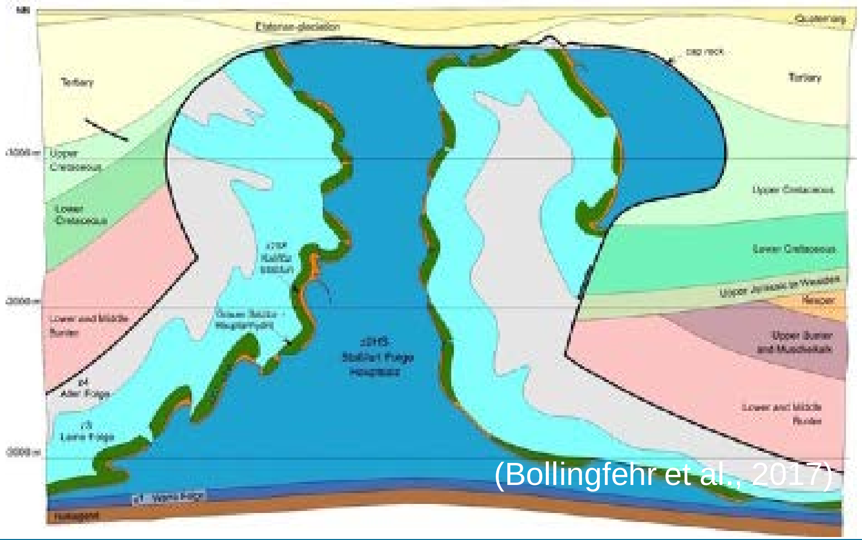
Task F Objectives – Comparison of Performance Assessment Models and Methods

Crystalline



SKB R-09-20

Salt Dome

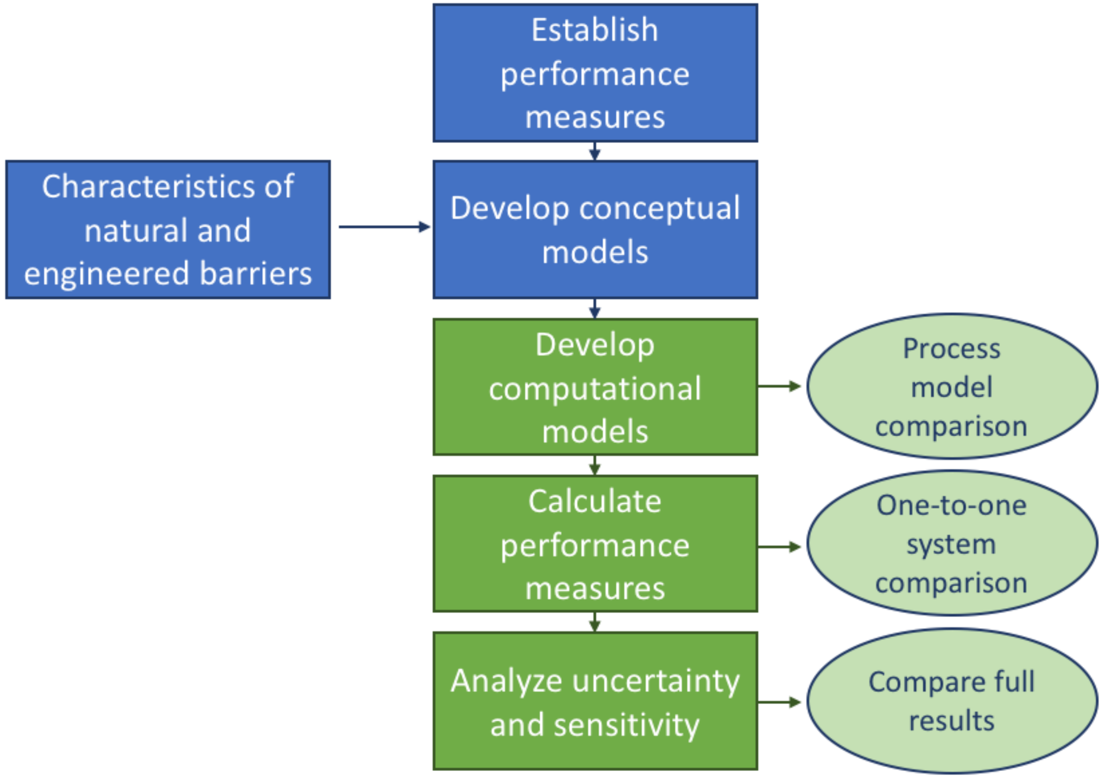


(Bollingfehr et al., 2017)

- 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 F 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 is Atypical

Typical DECOVALEX Task

Benchmarks

↓

Test cases

↓

Blind predictions

↓

Applications

Task F

Benchmarks

↓

Applications

Teams

Crystalline

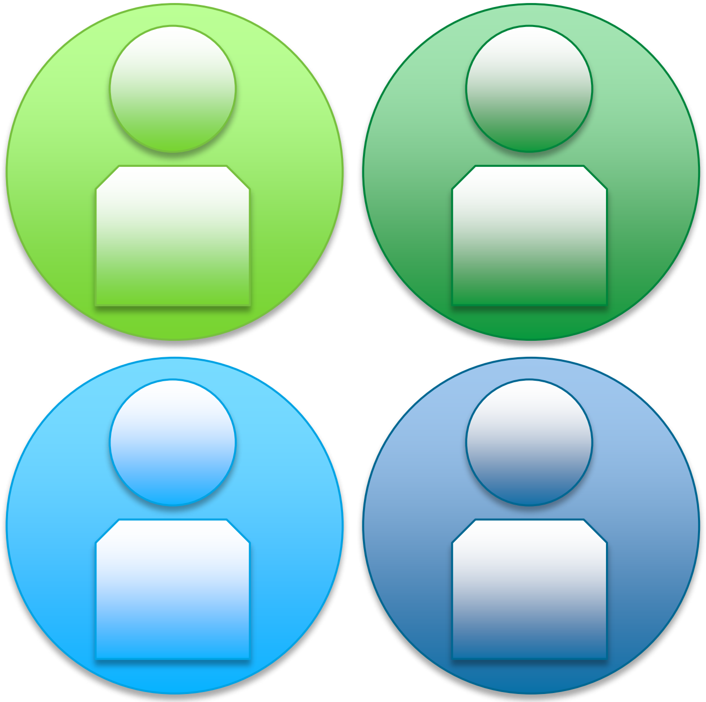
Canada REGULATOR	Canada IMPLEMENTER	Czech Republic IMPLEMENTER	Germany GEOSCIENCE ADVISOR	Germany REGULATOR	Germany SAFETY CONSULTANT	Korea IMPLEMENTER	Sweden REGULATOR	Taiwan IMPLEMENTER	United States IMPLEMENTER

Salt

Germany REGULATOR	Germany SAFETY CONSULTANT	Netherlands IMPLEMENTER	United Kingdom SAFETY CONSULTANT	United States IMPLEMENTER

Benefit to Program

- Integration of features and processes
  - Generation and upscaling of discrete fracture networks
  - Dual continuum fracture-matrix diffusion
  - Salt reconsolidation
- Confidence building
  - Software benchmarking
  - Comparison of modeling approaches
  - Mutual learning
- Next generation of repository scientists
  - Reference case development
  - Numerical implementation and simulation
  - PFLOTRAN software development
  - Uncertainty and sensitivity analysis



Crystalline Benchmarks

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

Crystalline Benchmarks and Test Cases

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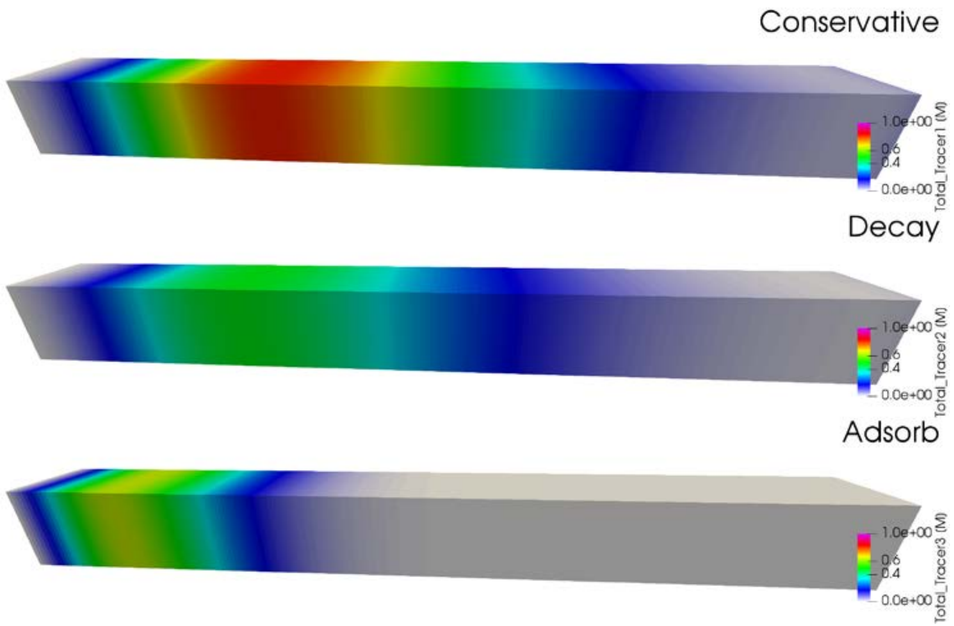
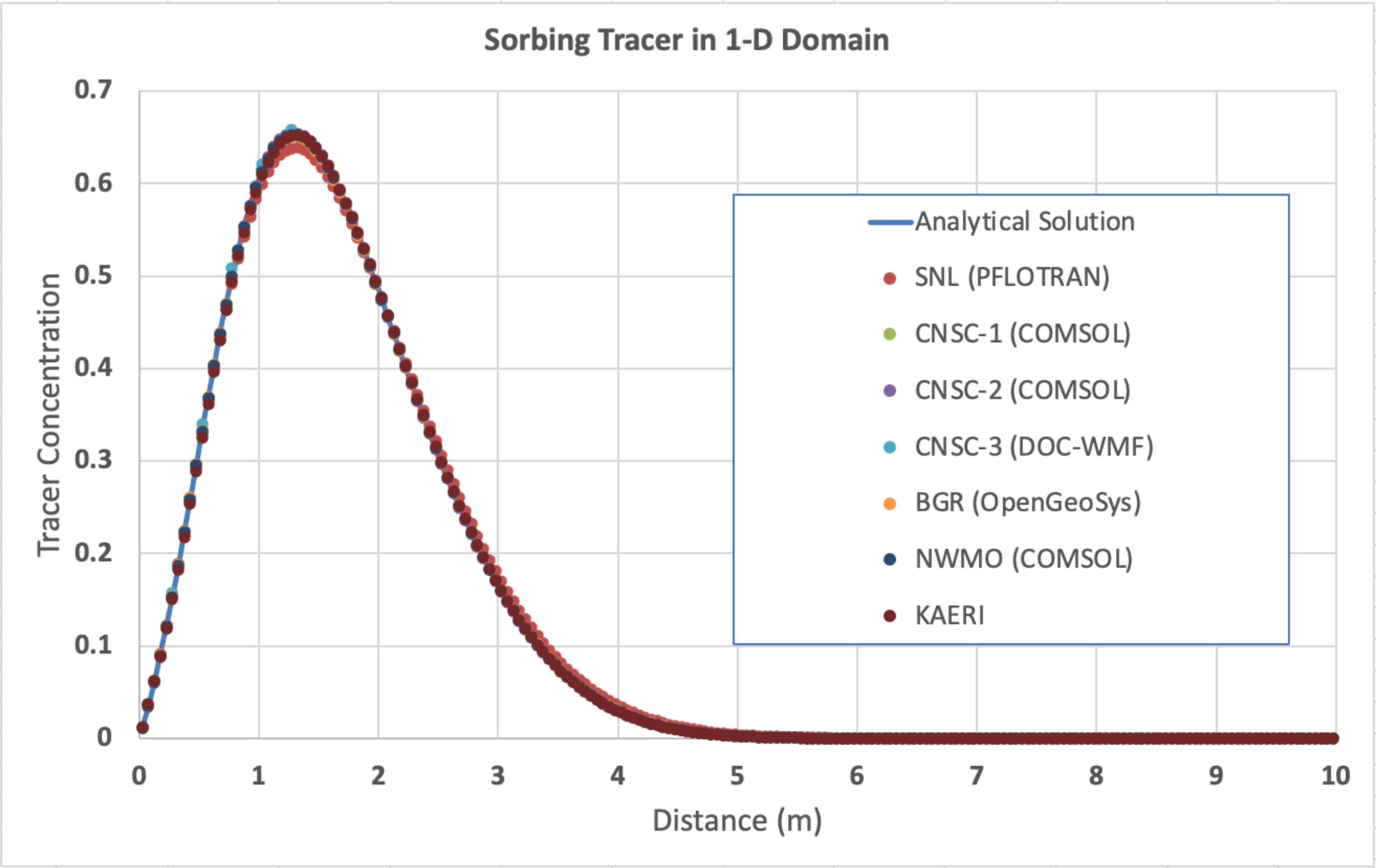
4-fracture network (deterministic)
Stochastic fracture network
Radionuclide source term
Buffer and canister processes

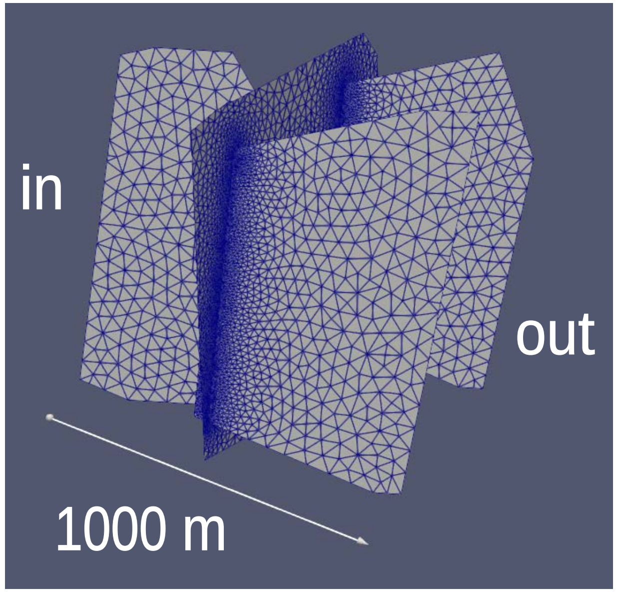
Transient Advection and Dispersion





- Conservative
- Decaying
- Adsorbing

4-Fracture Network



Discrete Fracture Network (DFN)

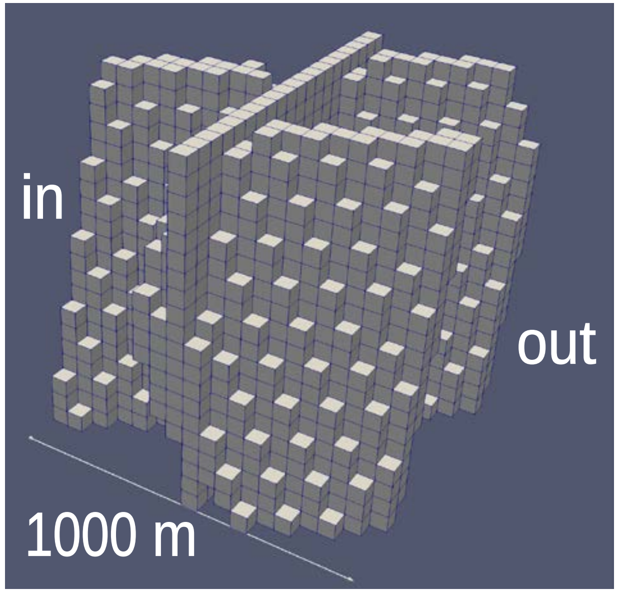
or

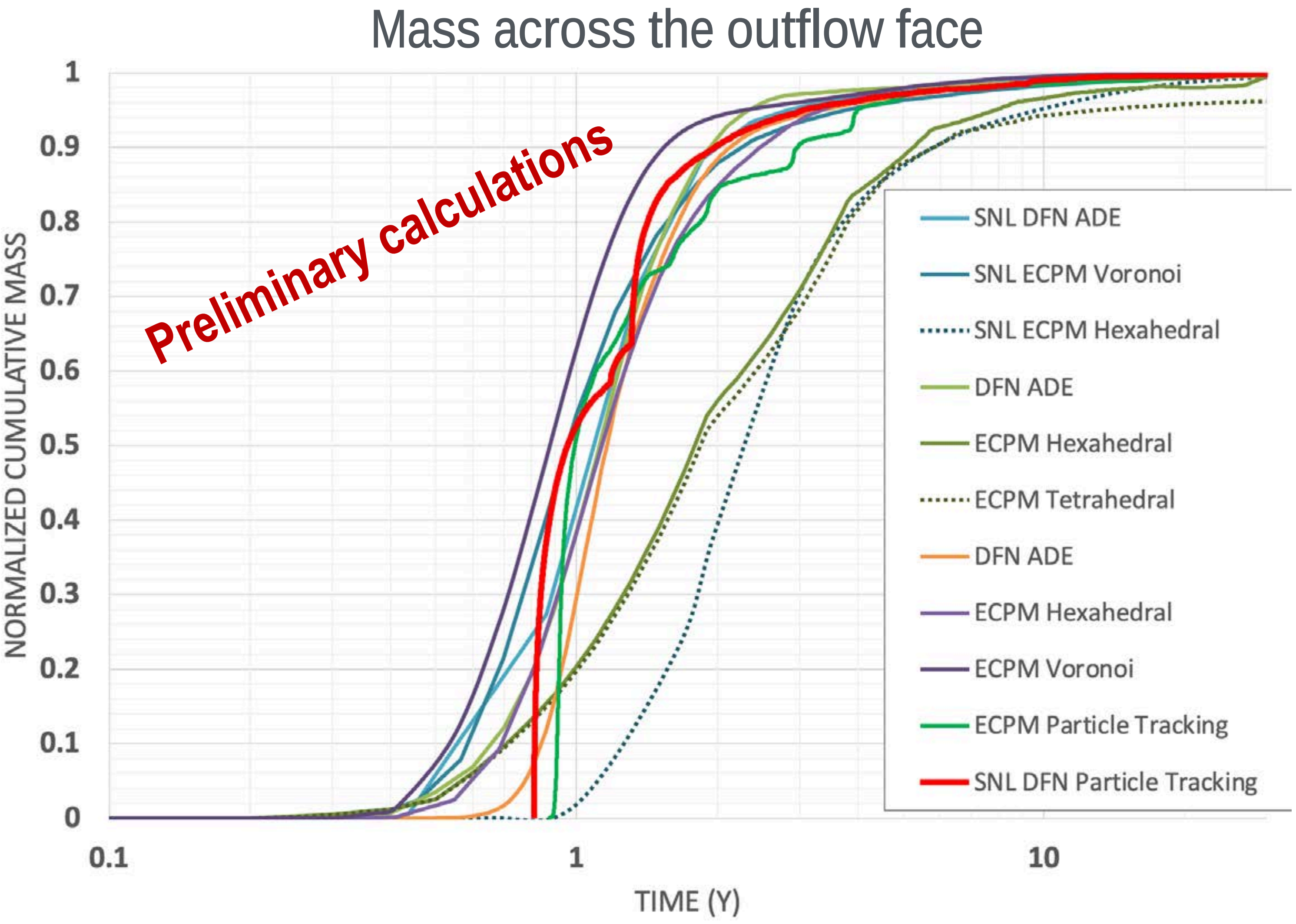
Equivalent Continuous Porous Medium (ECPM)

Particle Tracking

or

Advection-Dispersion Equation

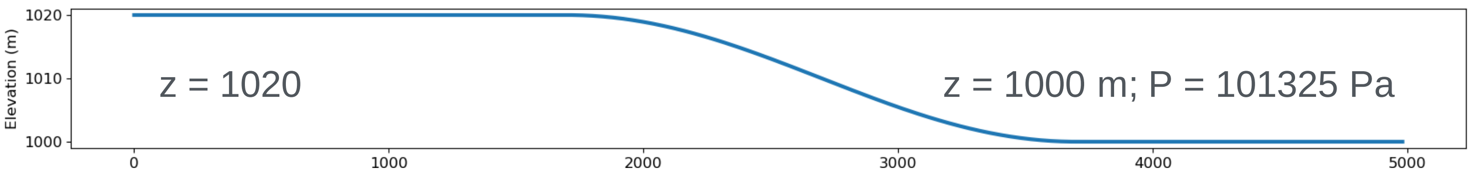


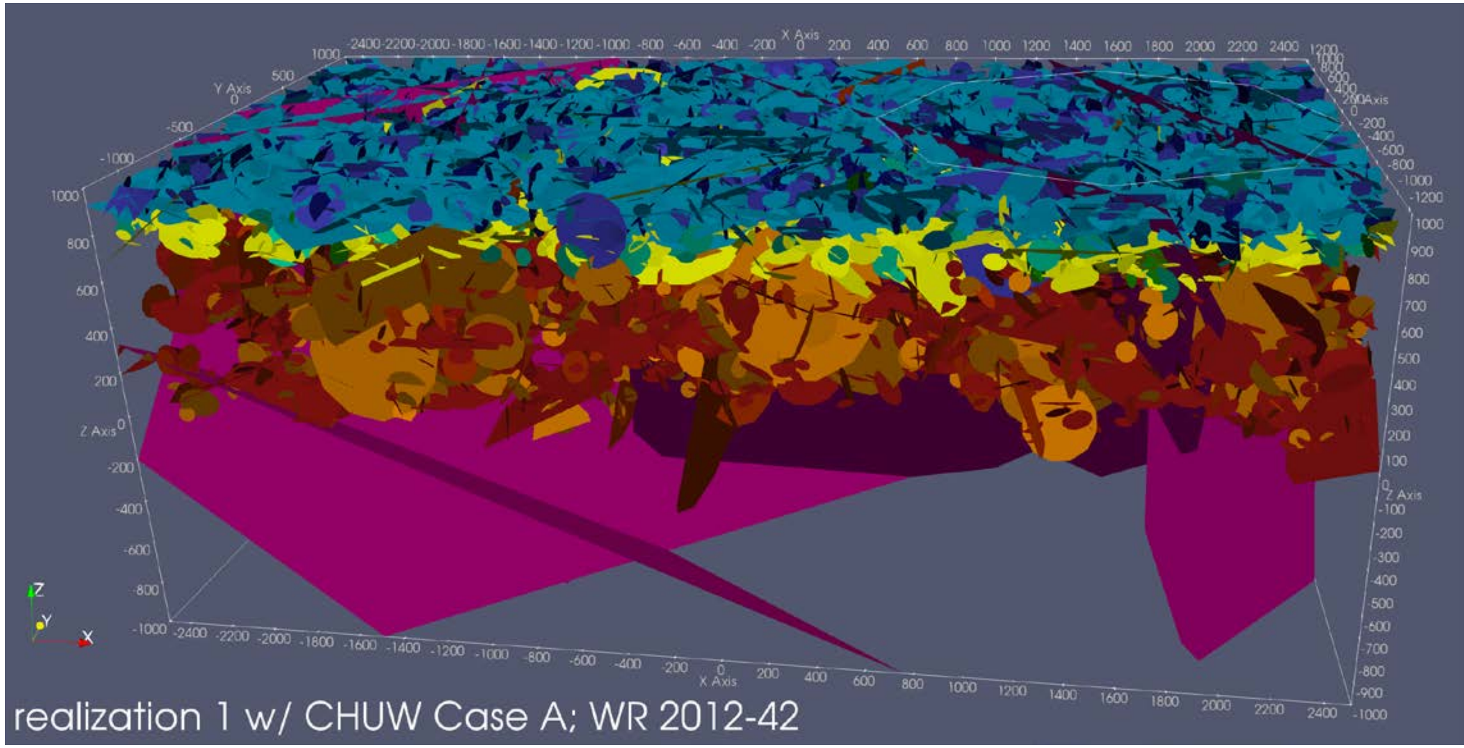


Crystalline Reference Case

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)





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

Initial simulations –

Tracer transport in steady state flow field

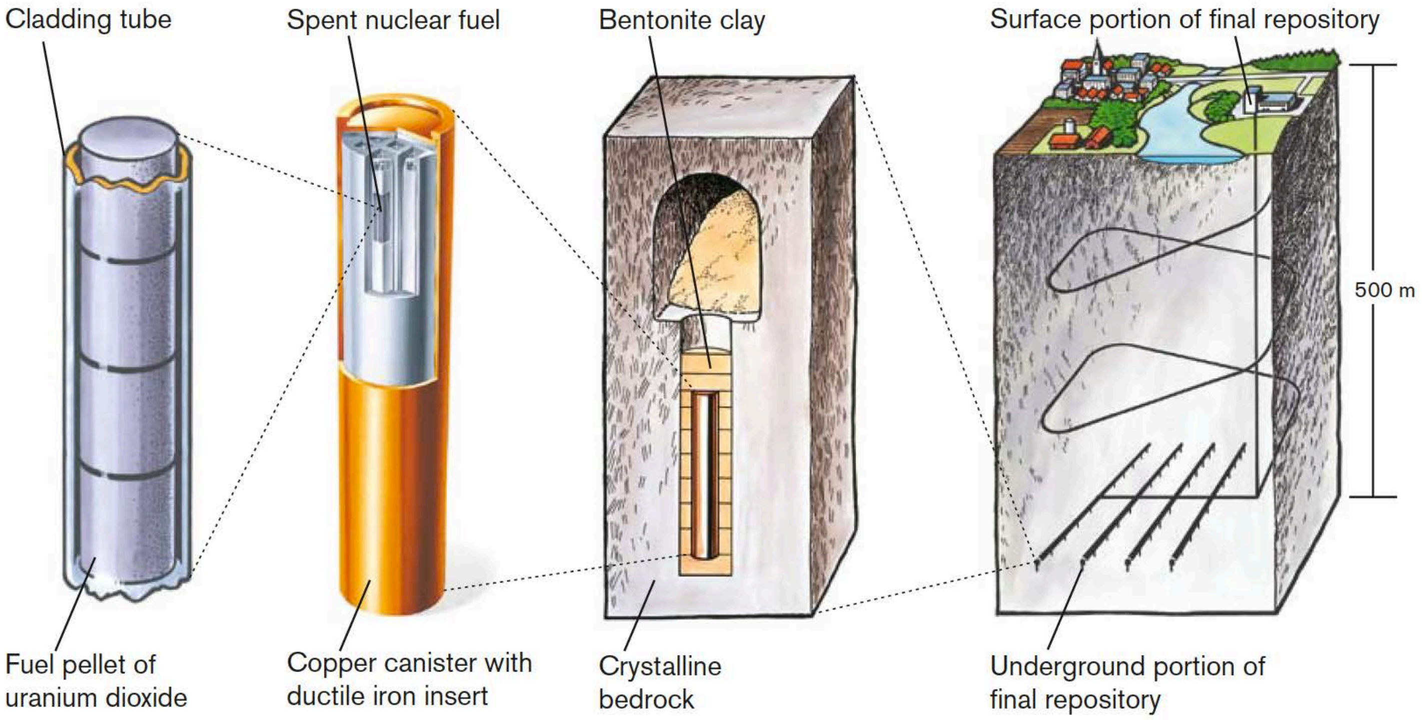


***Figure S-1.** The KBS-3 concept for disposal of spent nuclear fuel.*

Later Challenges – Canister Failure Mechanisms & Feedbacks

CANISTER FAILURE	Priority 1	2	3	4
Corrosion	3	4	-	1
Shear	2	2	4	-
Anything w/ glacial	3	1	-	4
Pinhole	2	1	2	2

Sorption models in buffer?

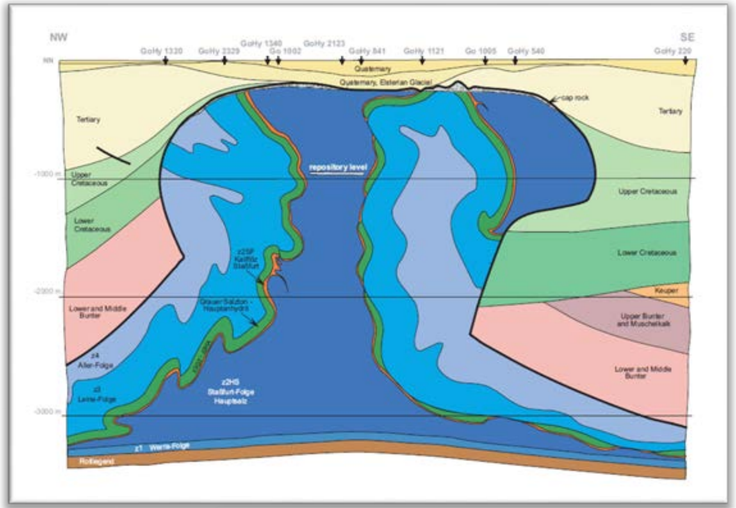
FEEDBACKS	Number of Interested Teams	Suggested Priority
Buffer erosion	6	1
Canister corrosion	4	1
Glacial on hydrologic boundary condition*	8	2
Glacial on Stress/Transmissivity	6	2 (optional)
Seismic on Stress/Transmissivity	4	-skip-
Thermal overpressure on transmissivity	5	1.5? (optional)

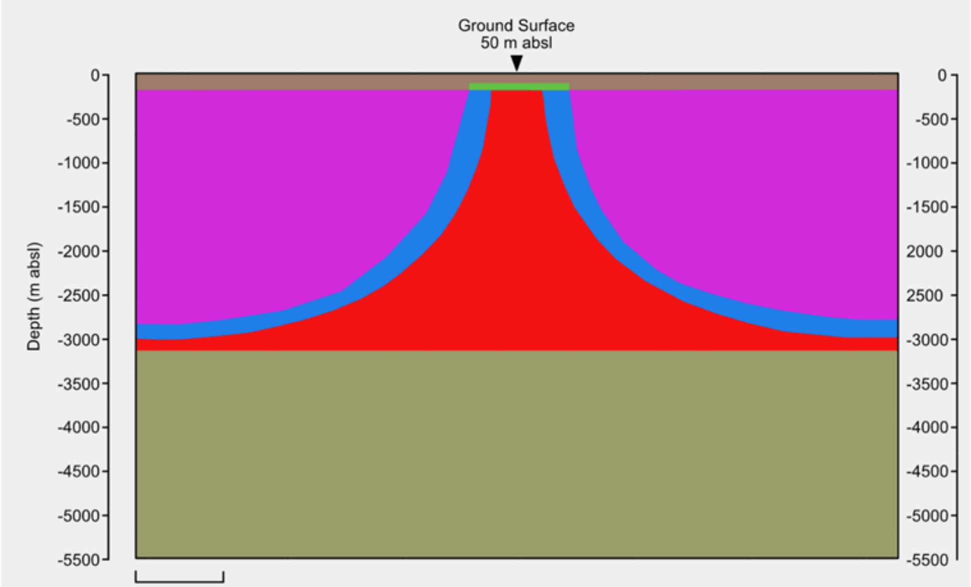
*and/or sea level change

Domal Salt Reference Case

Salt Reference Case – Natural Barrier System

- Salt dome
  - Low porosity ($\phi \leq\ 0.1\ \text{vol-\%}$)
  - Low permeability ($k \leq 10^{-22}\ \text{m}^2$)
  - No flowing groundwater ($\sim 0.1\ \text{vol-\%}$ brine)
  - High thermal conductivity ($\geq 5\ \text{W/m} \cdot \text{K}$)
  - Openings creep closed ($> 10^0 - 10^2\ \text{yr}$)
  - Crushed salt heals to intact salt





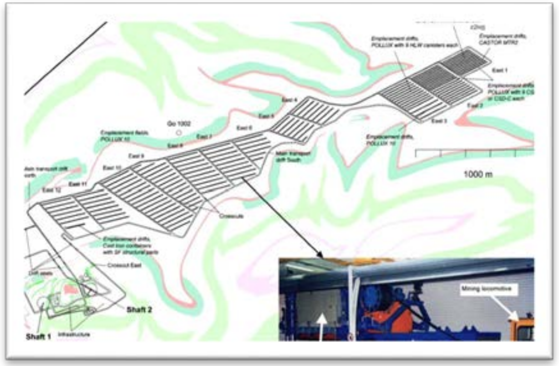
Courtesy of Jan Thiedau and Tatjana Thiemeyer

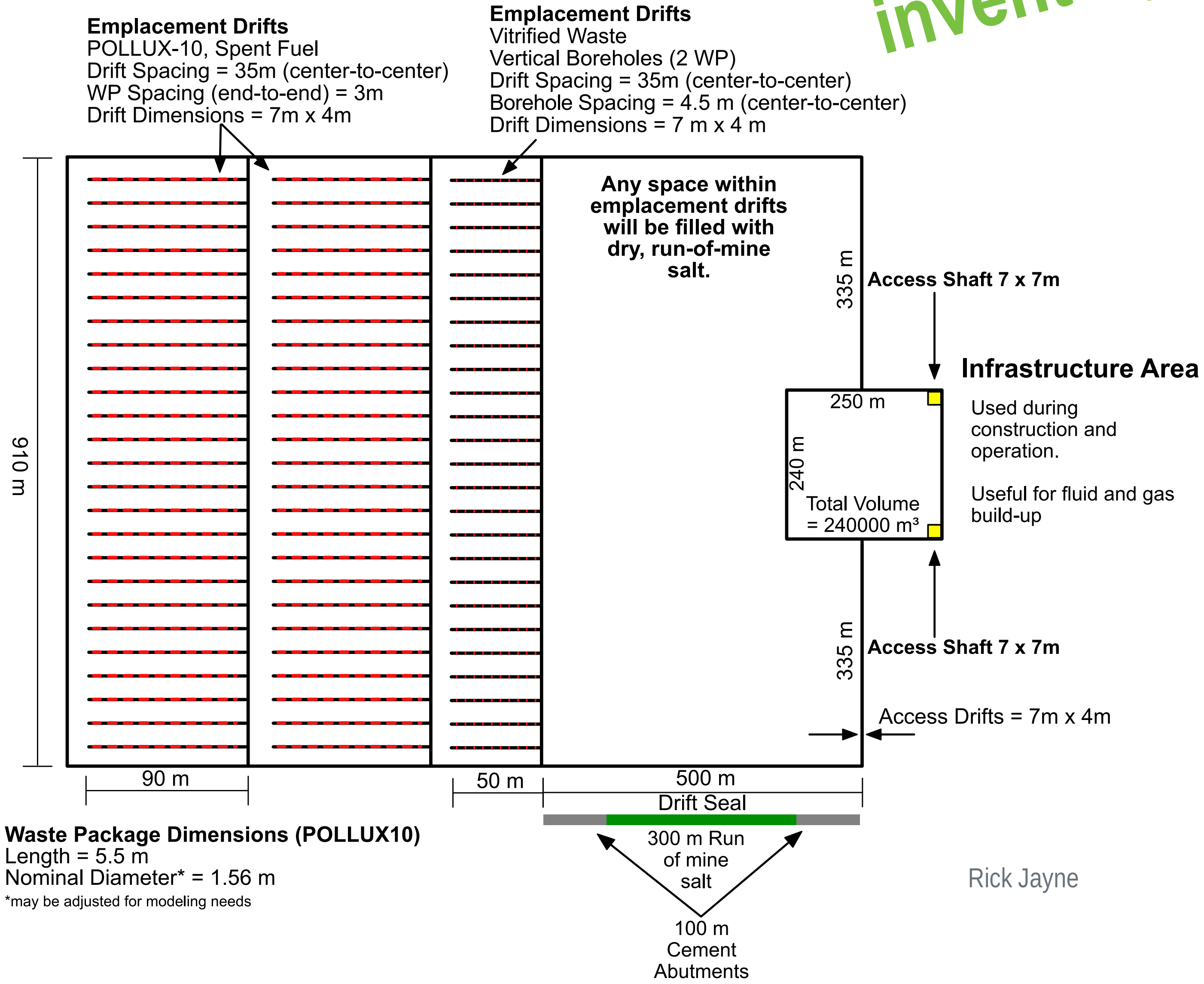
Simplified geometry

Salt Reference Case – Engineered Barrier System

Small inventory

- Features borrowed from Germany, Netherlands, United States
  - Glass waste form
  - Spent nuclear fuel
  - Cast iron canister
  - Crushed salt backfill in drifts
  - Gravel in infrastructure area
  - Drift seals
  - Shaft seals



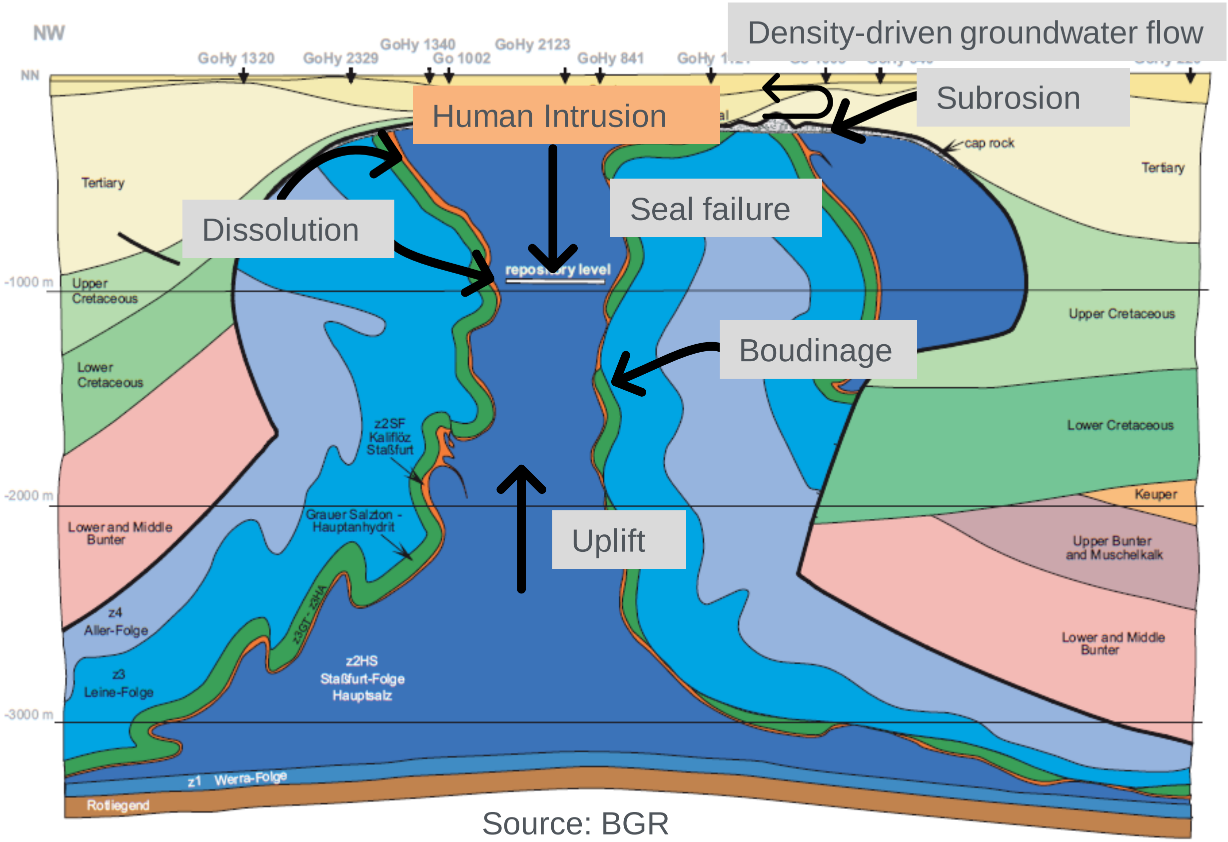


Rick Jayne

Staged Model Development for Shaft Seal Failure Scenario

- What if the shaft seals fail at 1000 y?
  - Modeled as permeability increase
- 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)

Failure scenario?

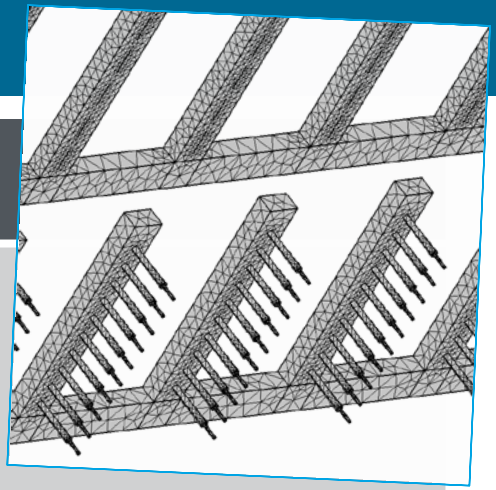


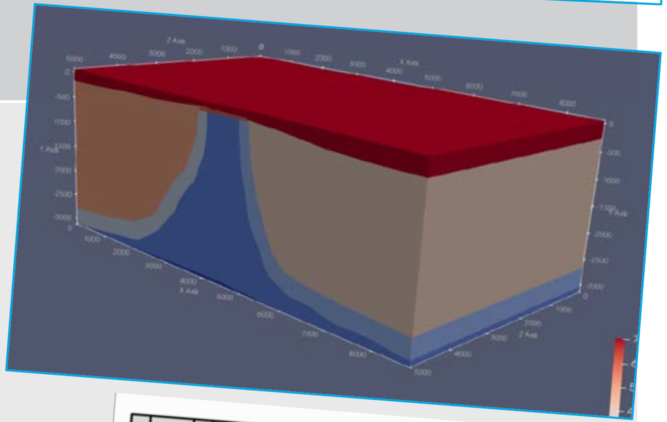
Source: BGR

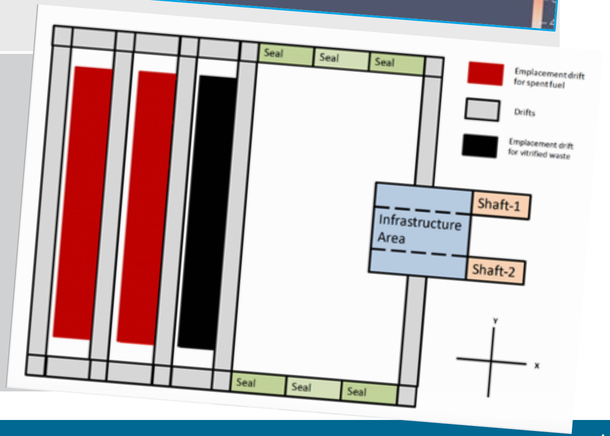
Jens Wolf, Salt Scenario Online Workshop 11-13 August 2020

Diverse Modeling Approaches

Team	Modeling Tool	Modeling Approach
COVRA NV	COMSOL	• Detailed representation of repository • Neglect impermeable host rock?
U.S. DEPARTMENT OF ENERGY	PFLOTRAN	• Geologic meshing • Include all volumes/materials
GRS global research for safety	LOPOS	• "Looped structures in repositories" • Segmented model







Summary

- Comparison of performance assessment models and methods
  - Crystalline and salt reference cases
- Build confidence
  - Address uncertainty introduced by modeling approach
  - Incorporate features, events, and processes identified in international programs
- Develop
  - Simulation and analysis capability
  - Next generation of repository scientists

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