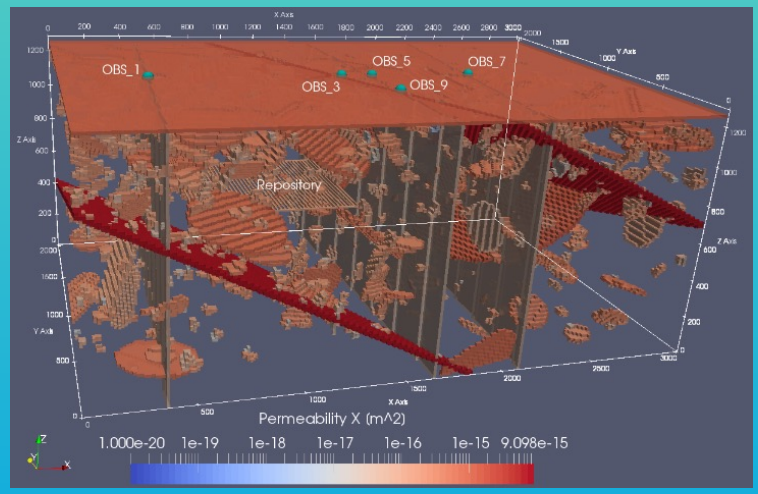
SAND2021-14419PE

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

Spent Fuel and Waste Science and Technology (SFWST)

Clean. Reliable. Nuclear.



DECOVALEX-2023 Task F (Performance Assessment) Synthesis, 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 the modeling teams

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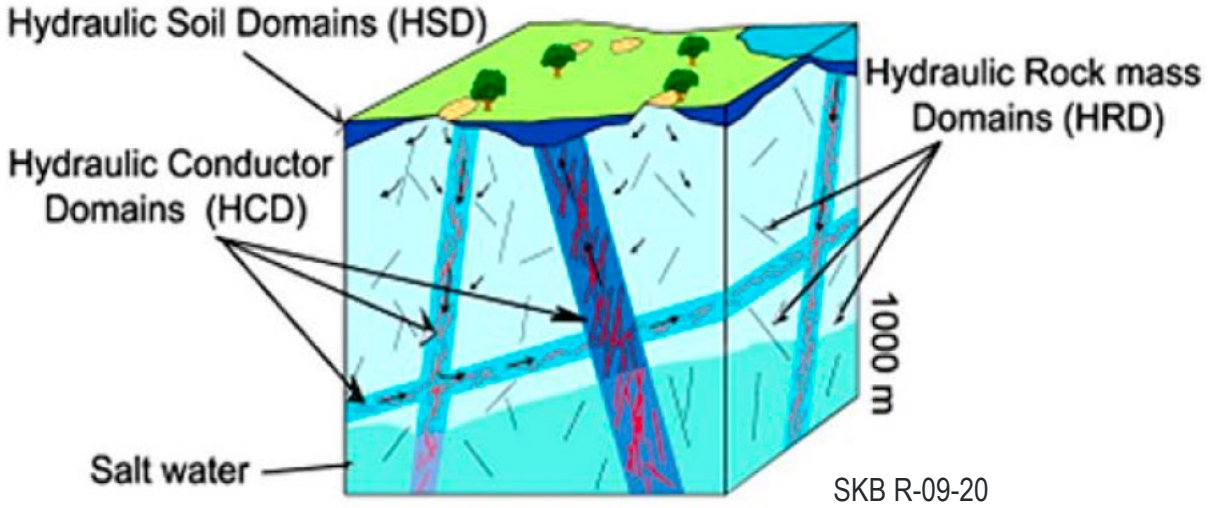
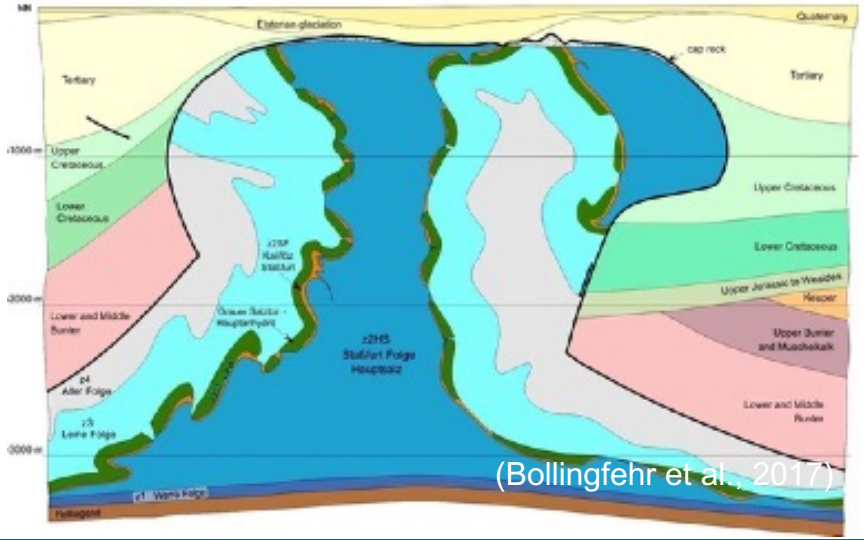
Task Objectives – Comparison of Models and Methods

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
  - Conceptual uncertainties

Crystalline

Task F1

Wednesday, 10 November

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

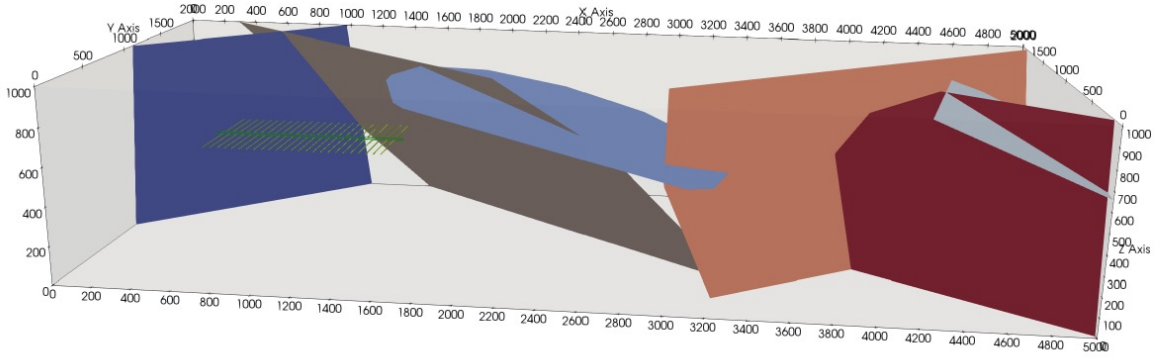
Start	Finish	Duration	Topic	Speaker
5:00	5:10	10	Welcome	Emily Stein
5:10	5:30	20	Structural Geology - Look ahead	Carlo Dietl
Presentations re '4frac' and '4frac+ revised' benchmarks:				
5:30	5:45	15	DOE	Rosie Leone
5:45	6:00	15	KAERI	Yong-Min Kim
6:00	6:15	15	INER/Taipower	Chieh-Chun Chang
6:15	6:30	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	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

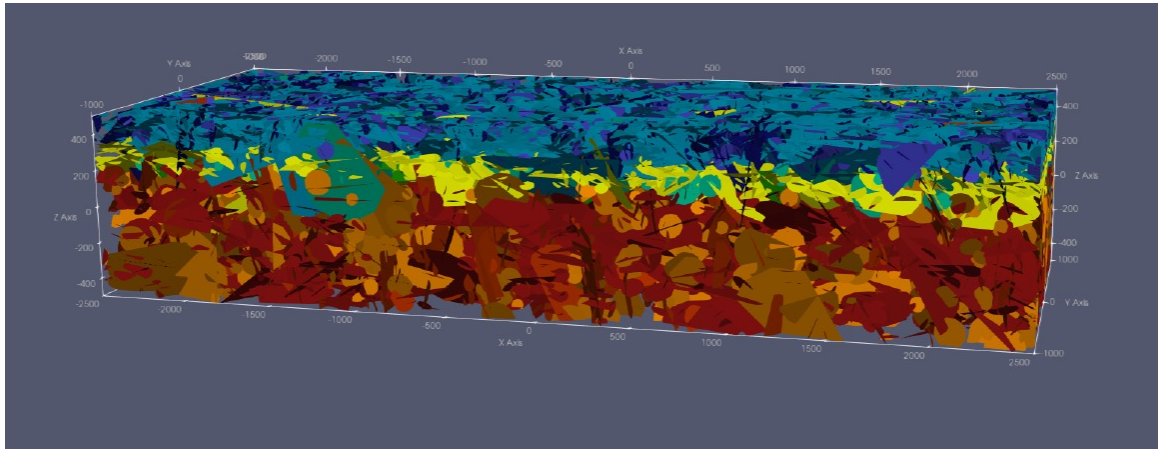
Benchmarks Accomplished

Team	Steady flow	1D transport (conservative, decaying, sorbing tracers)	Matrix diffusion (decaying tracer, two flow velocities)	4-frac (conservative tracer)	4-frac+ (conservative, decaying, sorbing tracers)	4-frac+ revised (conservative, decaying, sorbing tracers)
CNSC		✓	✓	✓	✓	✓
NWMO	✓	✓	✓	✓	NA?	NA?
SURAO	✓			✓	✓	✓
BGR		✓		✓		
KAERI	✓	✓	✓	✓	✓	✓
INER/TaiPower				✓		✓
SSM						
DOE	✓	✓	✓	✓	✓	✓

GRS, BASE, Quintessa not included on table.

Initial Reference Case





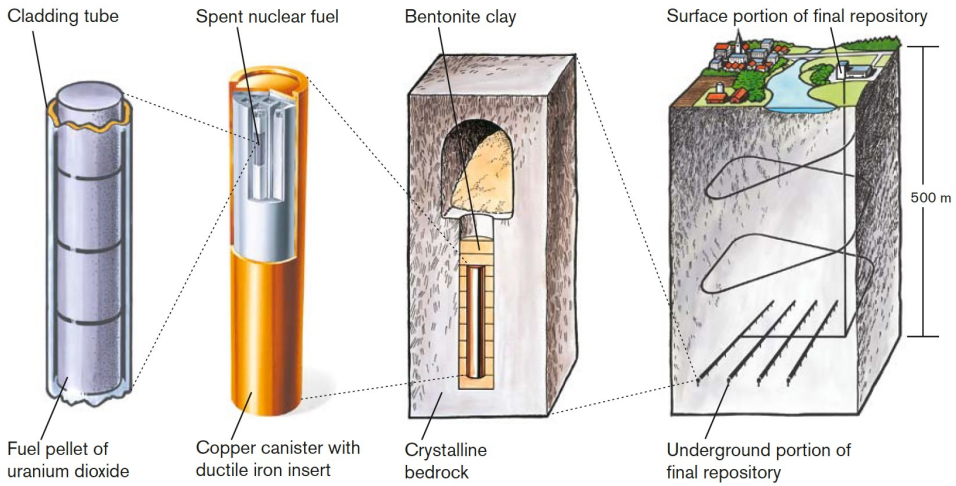


Figure S-1. *The KBS-3 concept for disposal of spent nuclear fuel.* SKB TR-11-01

Table 3-6. Tracer inventories and release mechanisms for initial reference case simulations.

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

Compare effective permeability and porosity of realizations

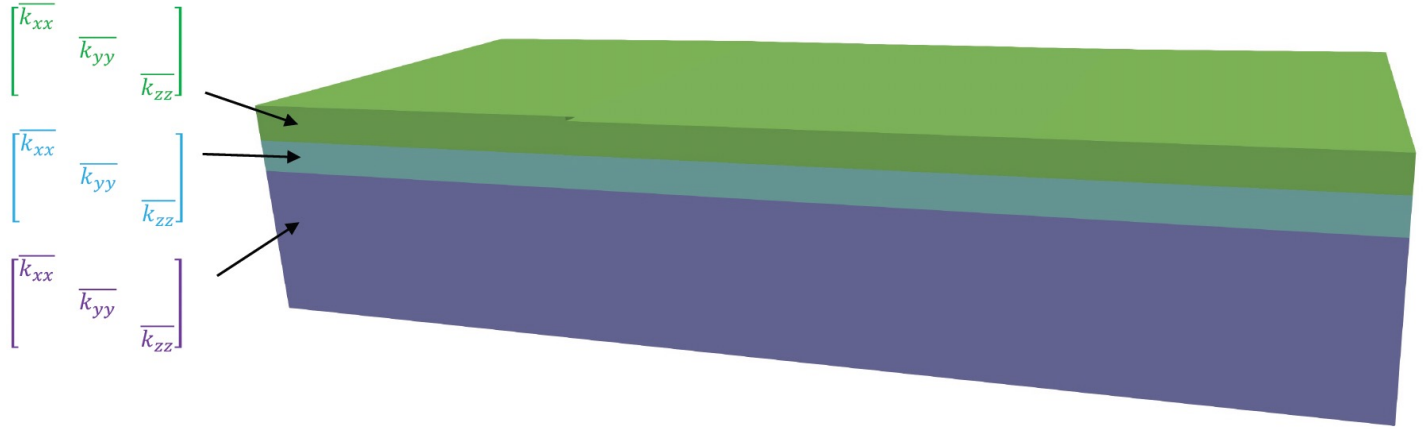
4 Deriving bulk permeability statistics

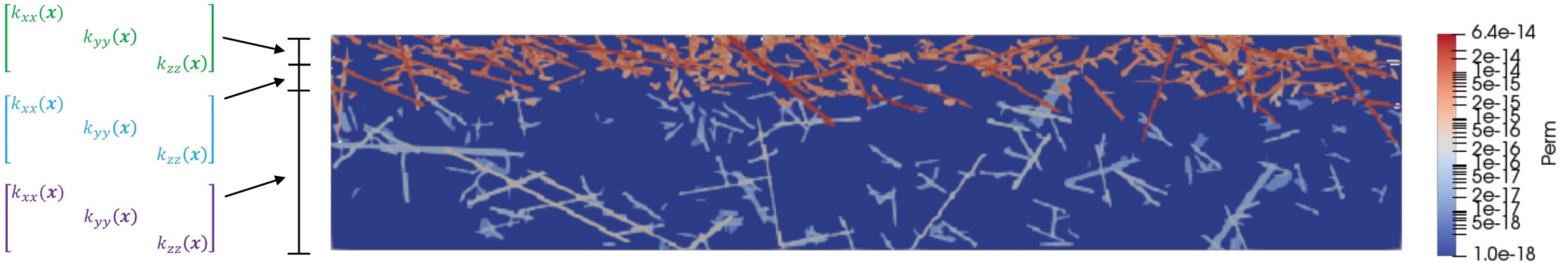
- Goal: compute bulk permeabilities for models assuming homogeneous subsurface properties by depth zone.
- Have spatially-varying $(\boldsymbol{x} = (x, y, z))$ random realizations of $k_{xx}(\boldsymbol{x}), k_{yy}(\boldsymbol{x})$, and $k_{zz}(\boldsymbol{x})$ from ECPM.

Compute subdomain-averaged permeabilities, e.g.:

$$\overline{k_{xx}}^{a} = \frac{1}{N_{cells}} \sum_{i=1}^{N_{cells}} k_{xx}(\boldsymbol{x_i})$$

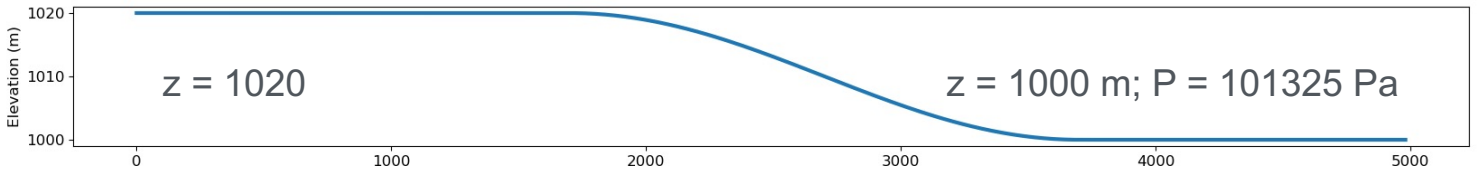
$$\overline{k_{xx}}^{g} = \left(\prod_{i=1}^{N_{cells}} k_{xx}(\boldsymbol{x_i}) \right)^{\frac{1}{N_{cells}}}$$

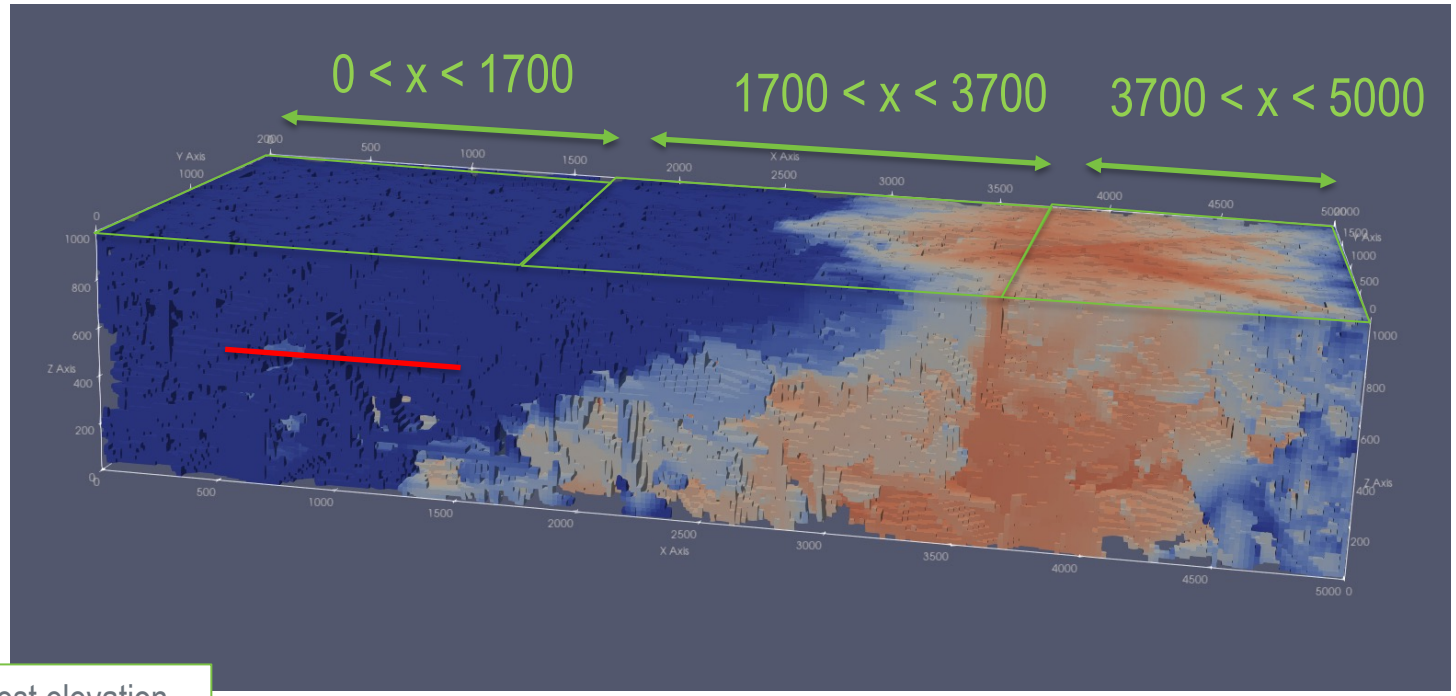




Compare liquid and tracer fluxes

- 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.

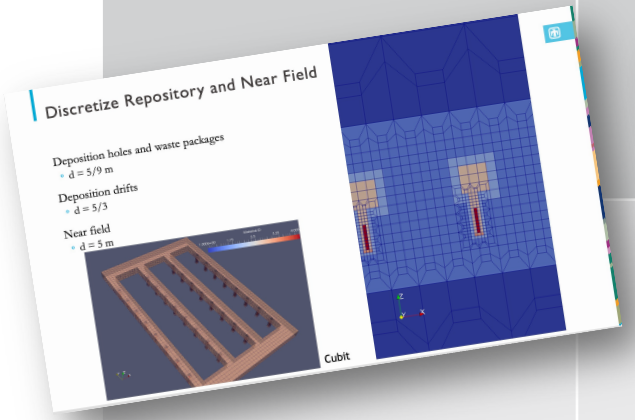


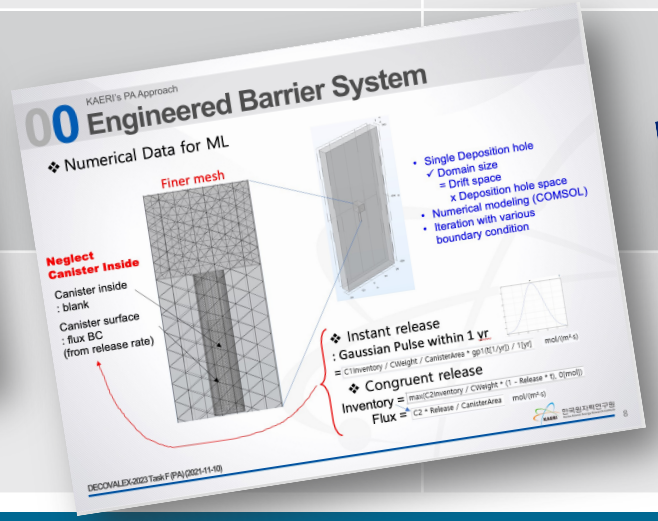


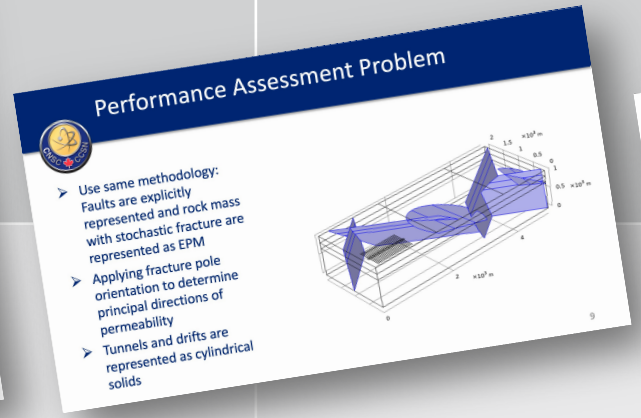
To be added to reference case: Find the location in the area of lowest elevation where the tracer mass flow is greatest. At this location …

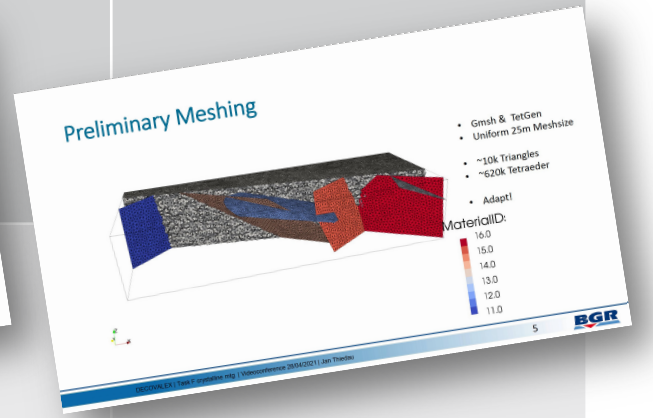
Reference Case Approach

DOE	INER/TaiPower	KAERI	CNSC	BGR
• dfnWorks • PFLOTRAN (FV)	• DarcyTools (FV) • GoldSim	• COMSOL (FE) • MATLAB	• COMSOL (FE)	• Fracman • OpenGeoSys (FE)
• ECPM • Advection-Dispersion Eqn	• 3D ECPM w/ particle tracking • 1D mass transport	• 2D planes in 3D porous medium • Advection-Dispersion Eqn	• 2D planes in 3D porous medium • Advection-Dispersion Eqn	• 2D planes in 3D porous medium • Advection-Dispersion Eqn









Schedule through Workshop 5

November ‘21	December ‘21	January ‘22	February ‘22	March ‘22	April ‘22
• dfnWorks output to teams who want it • What else?	• Template for interim report out	• Meeting to share and troubleshoot reference case simulations	• Interim report contributions due • Compile report	• Meeting? • Review, revise report	• Workshop #5 • Advance reference case • Interim report due

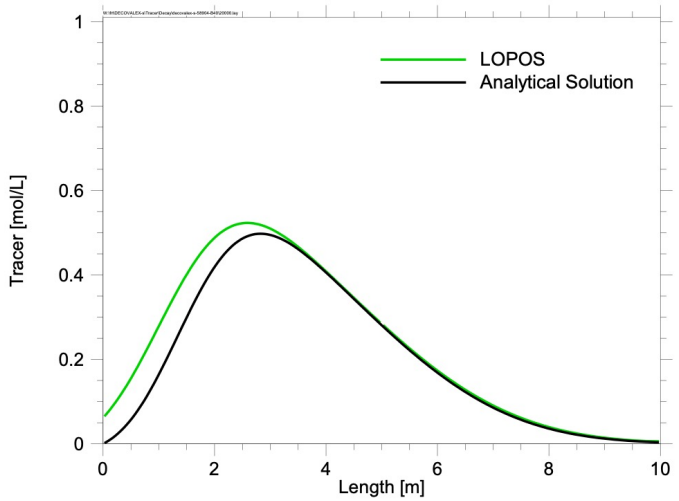
Salt

Task F2

Tuesday, 9 November

1D Benchmark Comparison

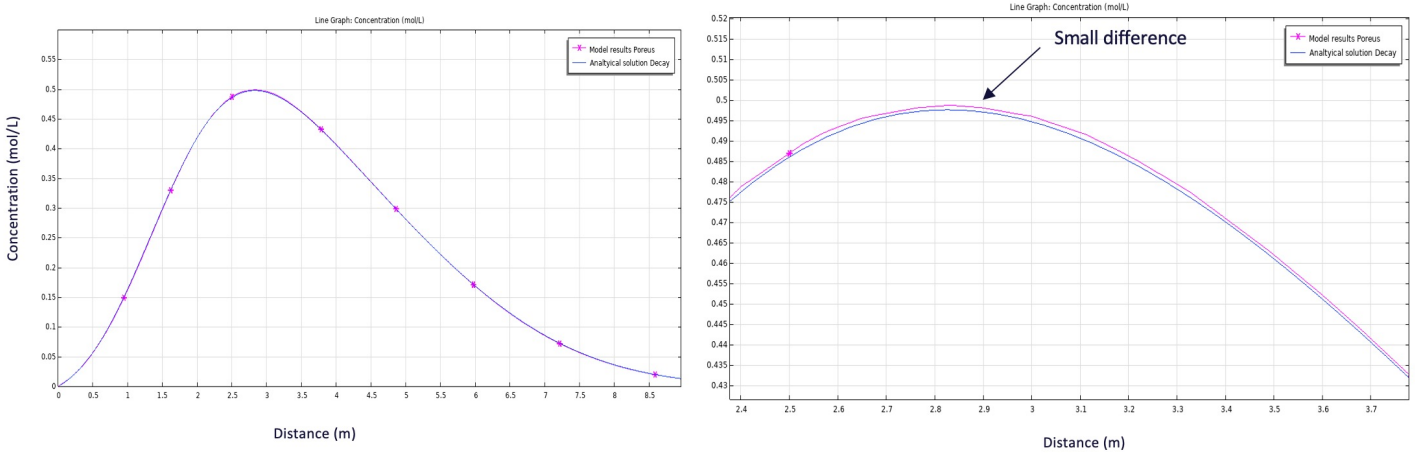
Decaying Tracer Decay constant: $5 \cdot 10^{-5}\ s^{-1}$



Frank et al. Task F2 presentation

BENCHMARK

Simple Transport + Decay Benchmark



Analytical solution from Kolditz et al ., (2015)

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www.covra.nl

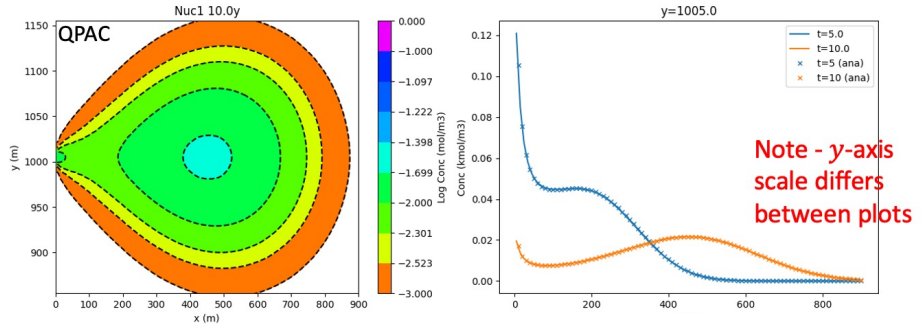
Bartol. Task F2 presentation

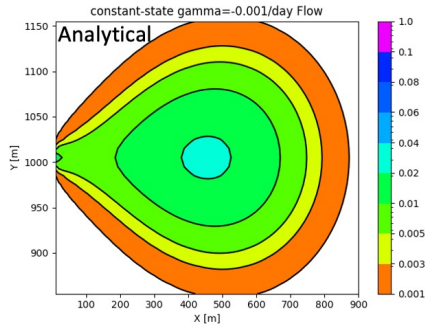
2D Benchmark Comparison

Case 3: No retardation, decaying source

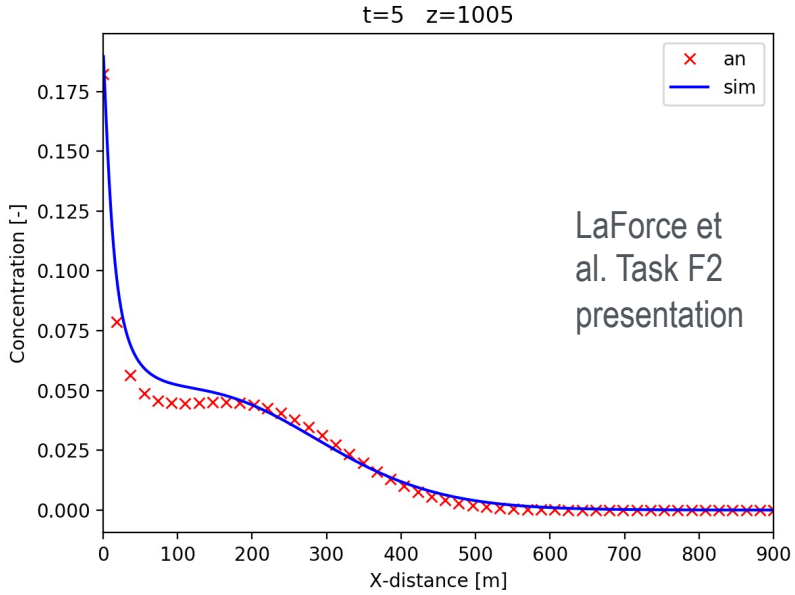
- Good match to analytical result

Benbow and Bond. Task F2 presentation



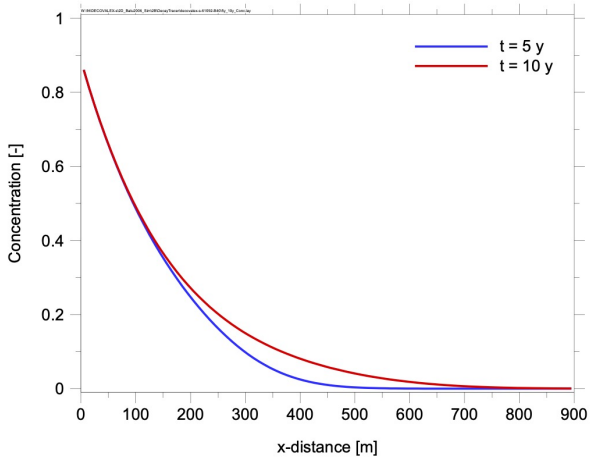


Values on QPAC colour bar are log conc.
Colours match in both cases



GeoTREND results for the decaying Tracer

z = 1005 m



Frank et al. Task F2 presentation

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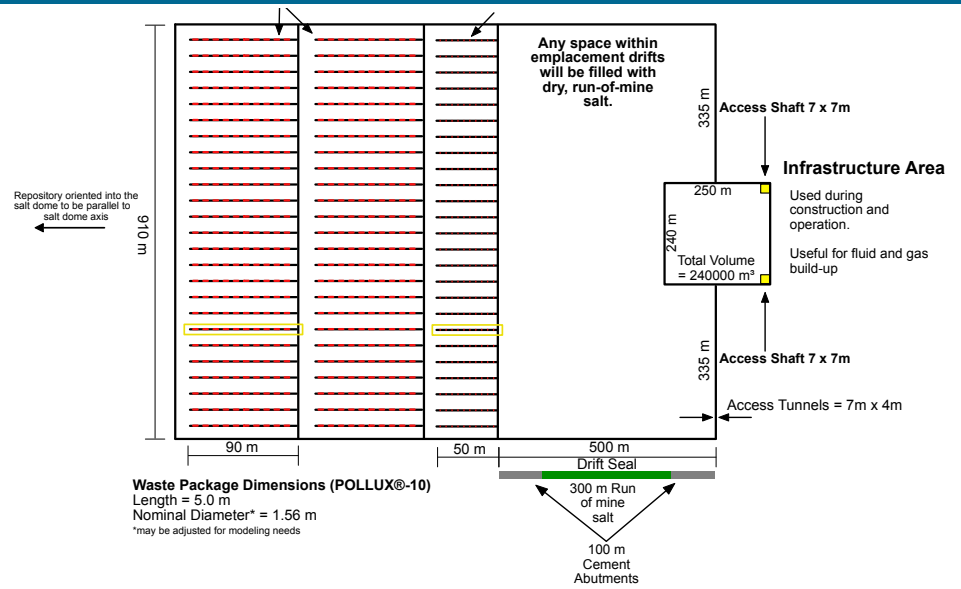
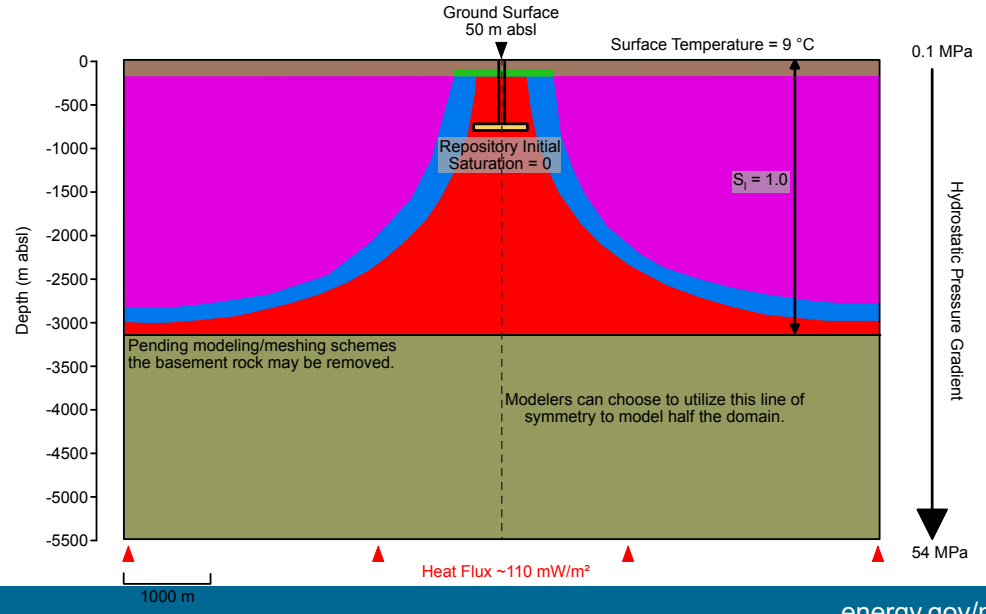
Shaft Seal Failure Scenario at 1000 yr

- Staged model development
  - Flow + radionuclide transport
  - + multiphase flow
  - + drift convergence
  - + heat flow and temperature-dependence of drift convergence
  - + model uncertainty in backfill consolidation model
  - (+ gas generation)
- Current task specification has sufficient information to construct model with
  - Multiphase flow and transport
  - Heat flow



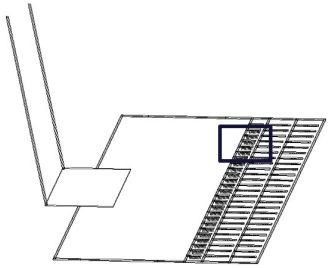


Modeling Approach

Team	Modeling Tools	Modeling Approach
COVRA	COMSOL	• Detailed representation of repository • Neglect impermeable host rock?
DOE (SNL/LANL)	PFLOTRAN	• Voronoi mesh • Include all geological volumes/materials • Simplified representation of repository
GRS	LOPOS, then later NaTREND	• "Looped structures in repositories" • Segmented model
Quintessa	GoldSim and QPAC	• Sequence of tank, 1D and 2D models linked together • Parallel implementation to study differences between codes

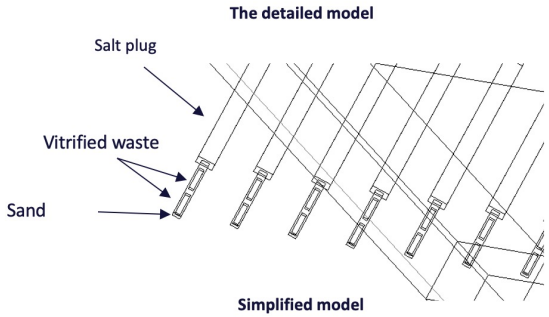
COVRA Modelling Concept

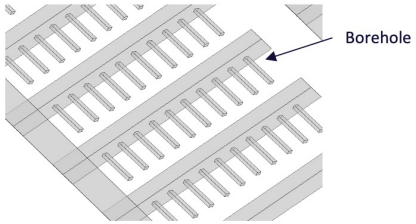
LAYOUT



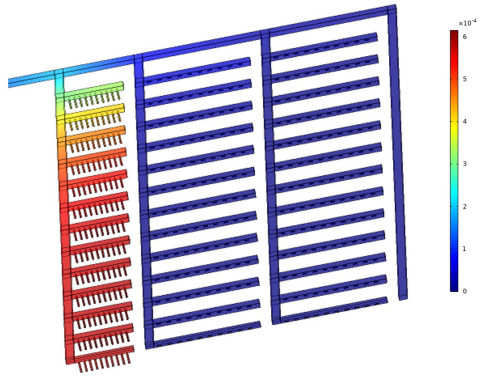
The setup presented during the **last conference was relatively detailed**. However, I had to simplify the model as the **mesh close to the vitrified waste was of poor quality**: the size of the elements was too large. Refining the mesh is possible but I opted to simplify the model domain.

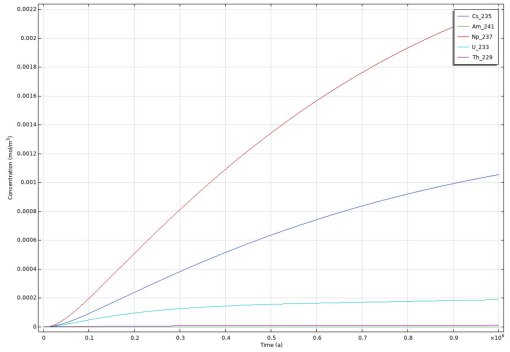
This simplification effectively assumes that the radionuclides enter the salt plug directly and not via the sand. Therefore, it is a conservative assumption.





EXPECTED RESULTS





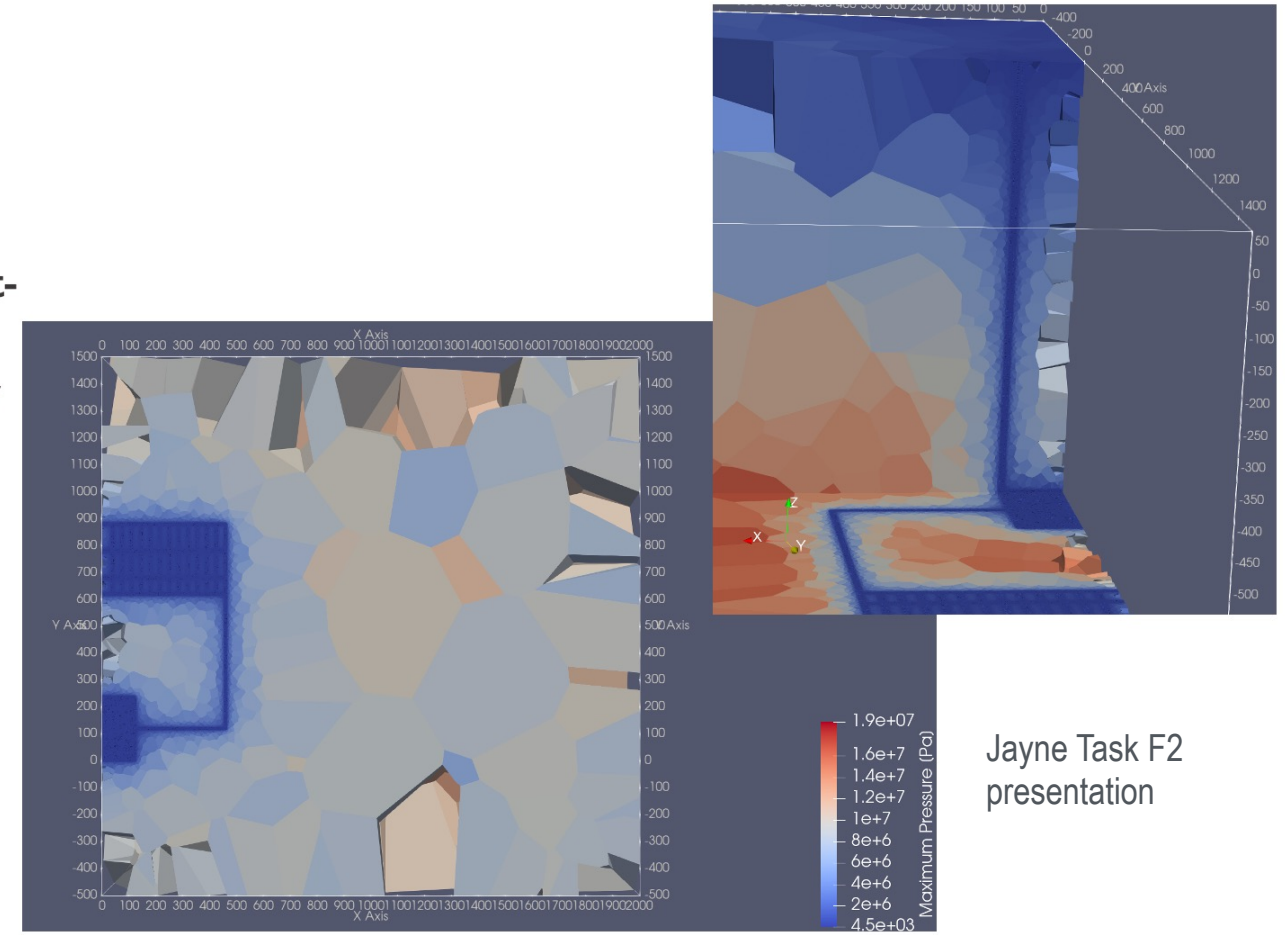
Bartol, Task F2 presentation

DOE (SNL) PFLOTRAN Modelling concept

100 Years – Pressure & Saturation – No Radionuclides

Grid cells are colored based on pressure at center of the grid cell

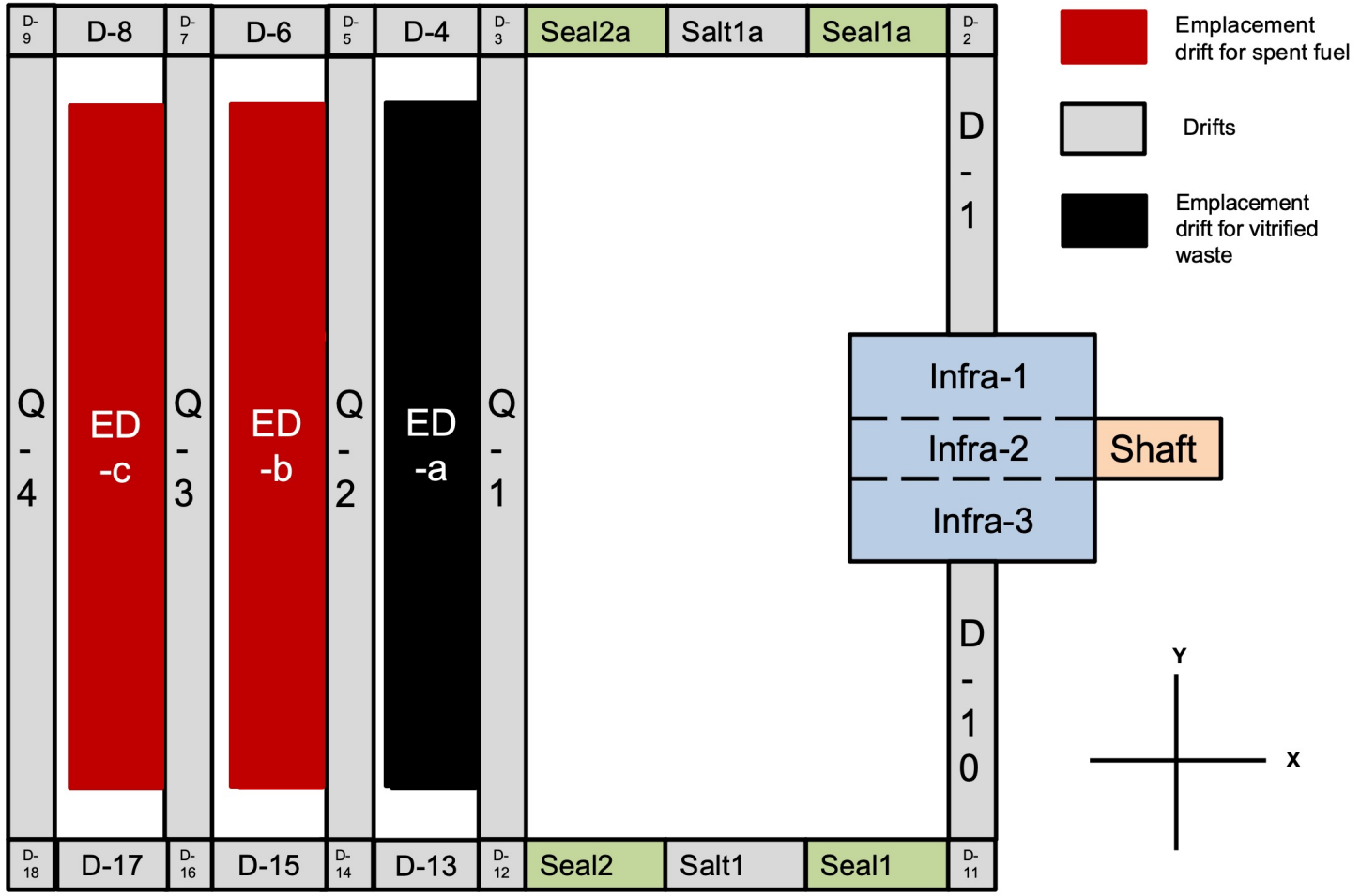
- Center of elements may be out-of-plane
- Higher resolution is most likely needed



Jayne Task F2 presentation

GRS LOPOS Modelling Concept

LOPOS Layout: simple emplacement drift design



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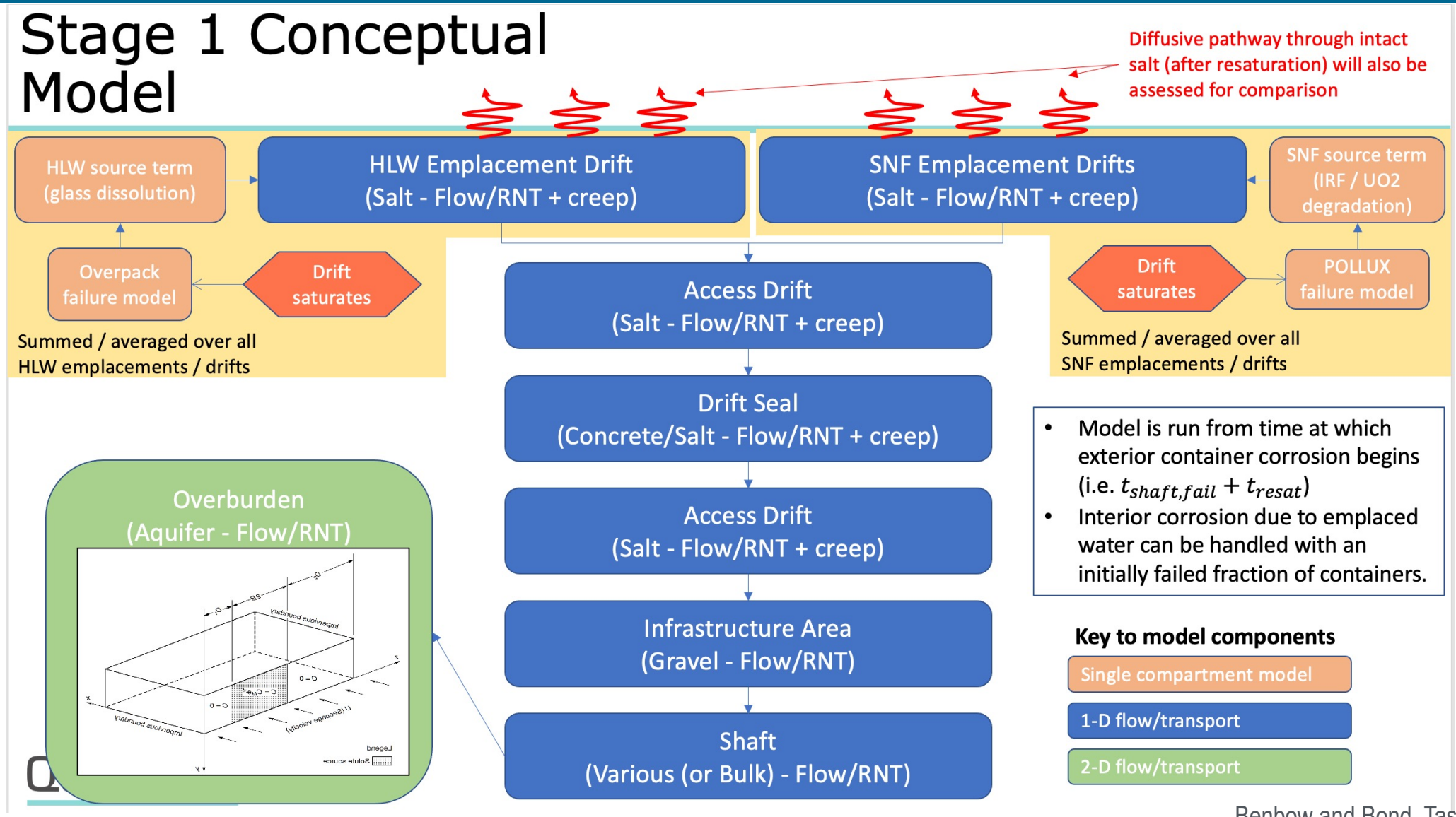
Quintessa Modelling Concept



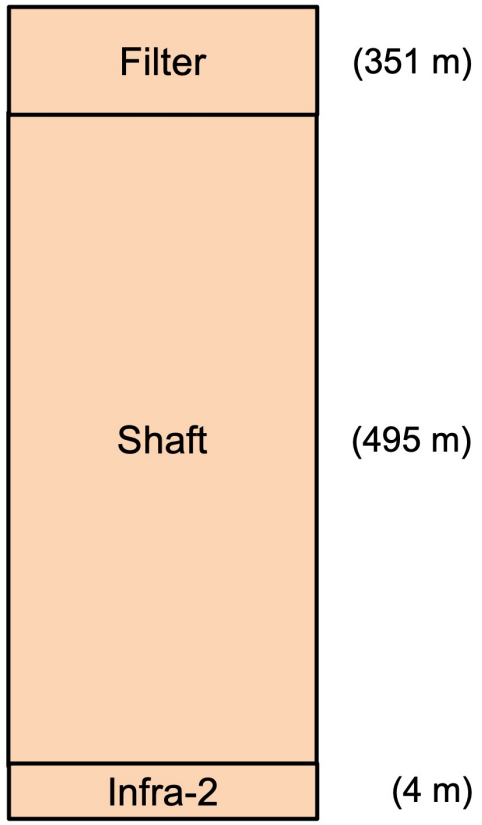
Benbow and Bond. Task F2 presentation

Lessons Learned

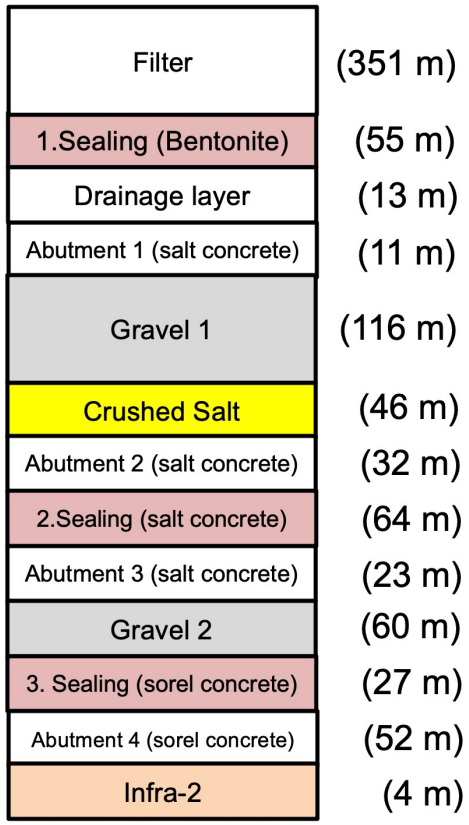
- Benchmarks
  - Useful to test ability of codes to model simplified problems
  - Raise the question of how good is good enough?
- Designing a reference case is an iterative process to create a case that is
  - Amenable to a variety of modeling approaches
  - Simple enough that we understand what we're comparing
  - Realistic, but also with potential for release so performance metrics can be tested

GRS

Shaft layouts



(GRS-415)



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Frank et al. Task F2 presentation

Next 6 Months

- Update task specification for full complexity shaft seals
- Teams finalize initial deterministic case simulations
- Comparison of initial simulation results

Schedule

Jan.	• Discuss progress on PA models. • Outline for interim report.
Feb.	• Collate team contributions to interim report • Begin to compare simulation results
March (tentative)	• Compare simulation results • Rough draft of interim report • Preparation and review for large meeting