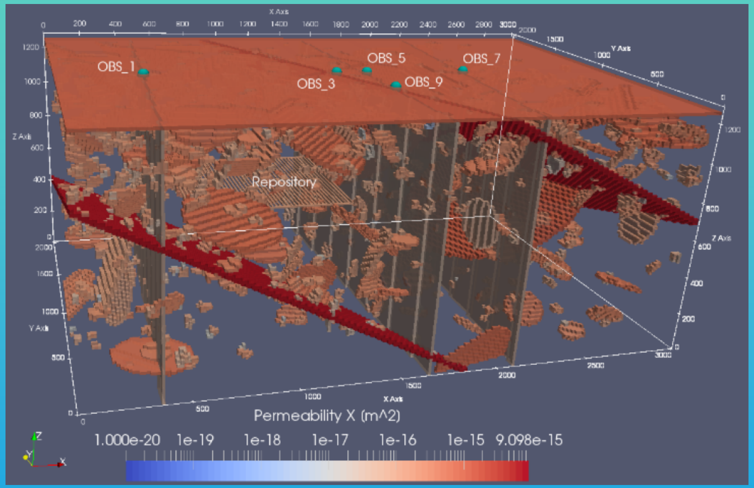
SAND2021-6148PE



DECOVALEX-2023 Tasks E and F

SFWST Day 4, DR Track
May 17-21, 2021
Virtual Workshop

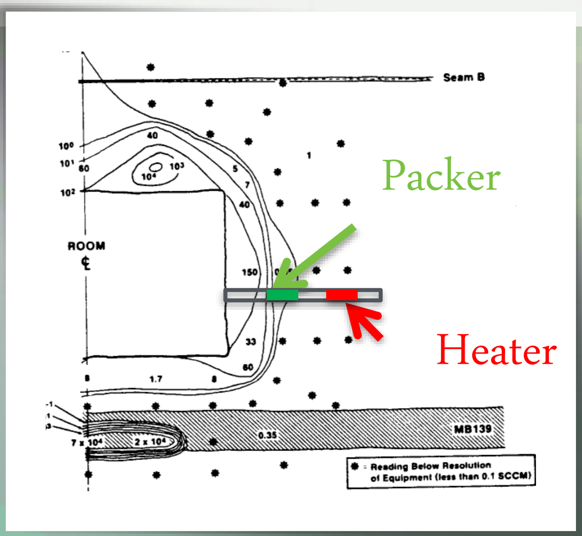
Emily Stein & Kris Kuhlman
Sandia National Laboratories

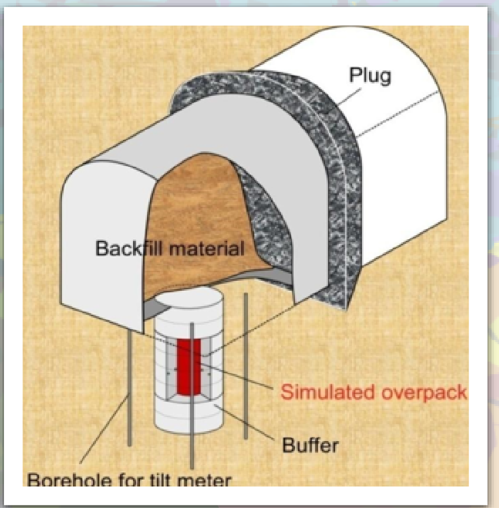
Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. Approved for unclassified, unlimited release ().

DECOVALEX – Development of Coupled Models & Validation against Experiments

Task E Lead
Brine Availability Test in Salt

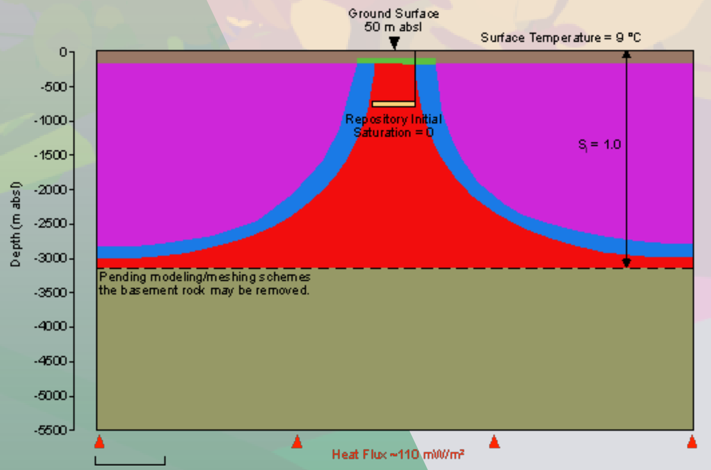
- 4 teams
- Predict and quantify coupled thermal, hydrological, mechanical and chemical processes





DOE Task Participation

- Gas transport in bentonite
- EBS Task Force
- HotBENT Experiments
- THMC Modeling
- FEBEX
- Mizunami GREET Experiment



Task F1 & F2 Lead
Performance Assessment

- 10 teams
- Compare models & methods
- Salt and Crystalline cases

- DECOVALEX-2023 has17 international partner organizations and features 7 tasks.

SFWST's participation in DECOVALEX grows capability and relationships.

https://decovalex.org

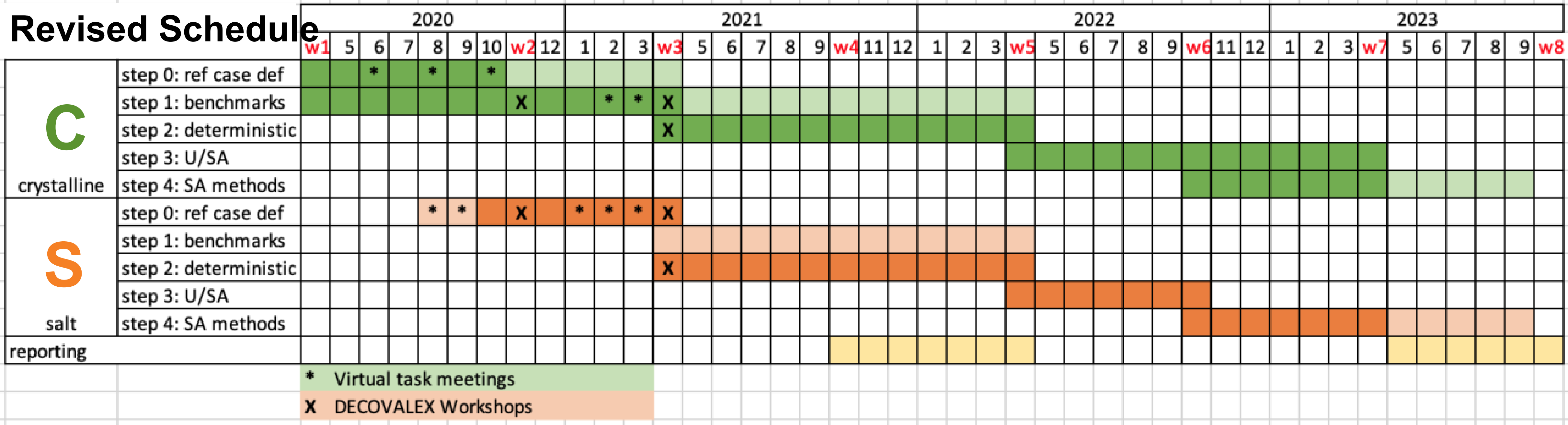
Additional benefits of leading tasks

- Problems are tailored to SFWST interests and needs
- Motivates capability development which can be coordinated with evolution of the DECOVALEX task
  - Fracture-matrix interaction
  - Particle tracking methods
  - Salt constitutive models (and implementation in PA)
- Extra bang for the buck – crowd-sourced returns are greater
  - More modeling approaches
  - More one-off analyses
- "Sells" open source software and recruits more code-breakers
  - dfnWorks
  - LaGrit
  - PFLOTRAN

DECOVALEX Task F

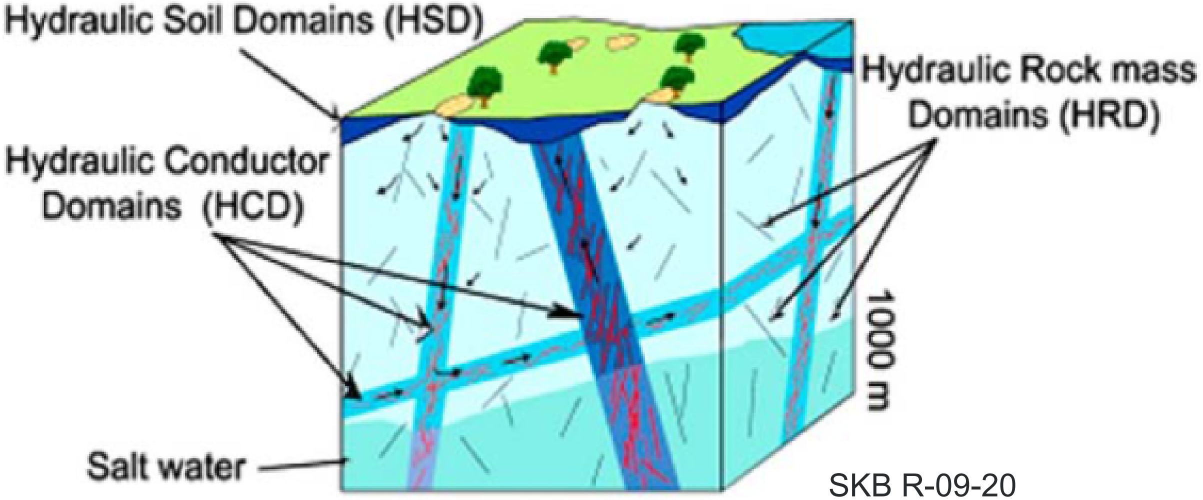
Performance Assessment

Revised Schedule



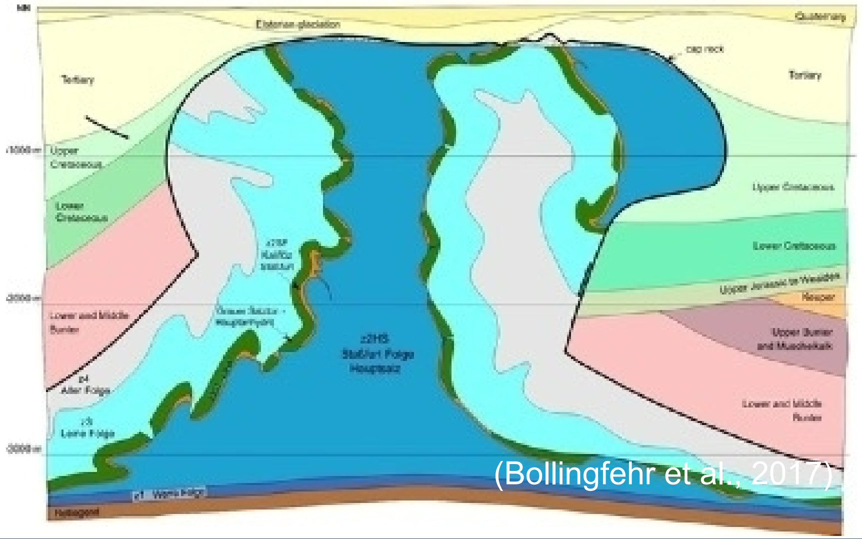
Task Objectives – Comparison of Models and Methods

Crystalline



SKB R-09-20

Salt Dome

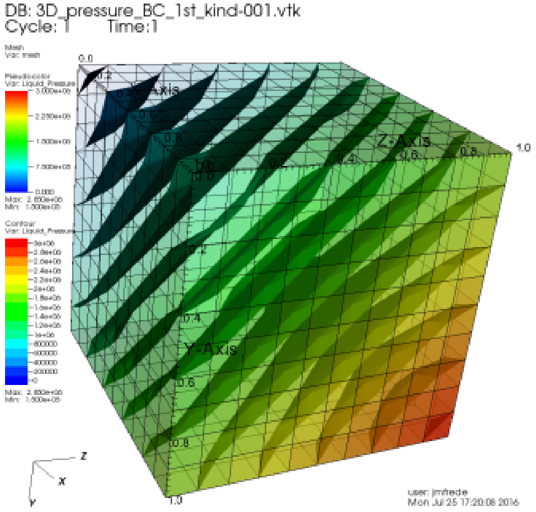


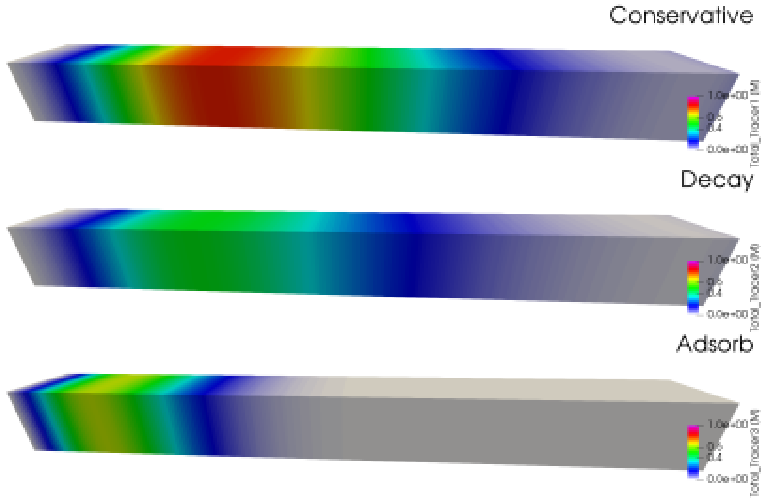
(Bollingfehr et al., 2017)

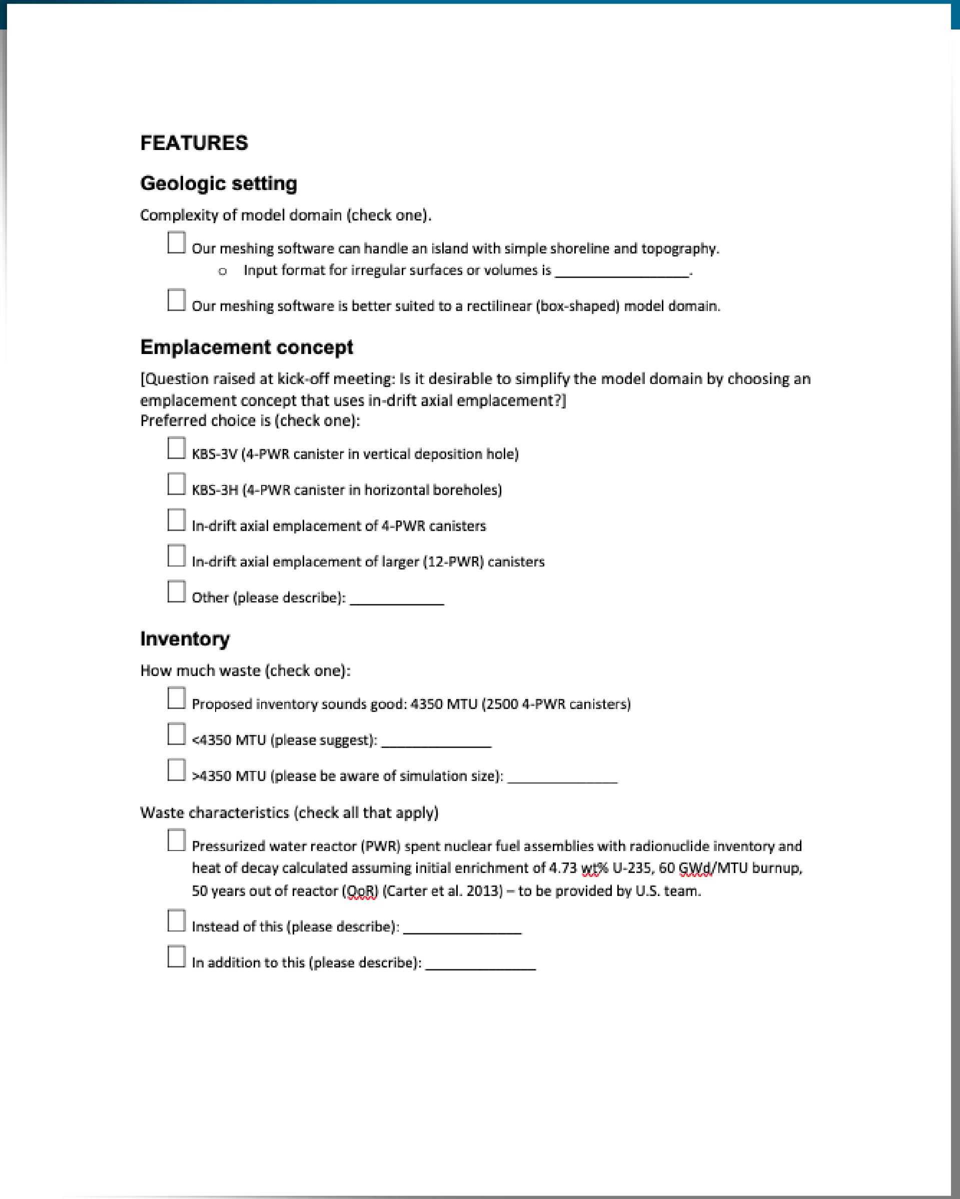
- Capability development
  - Software
  - Workflow
  - People
- Influence of modelling choices
  - Model fidelity
  - Omission/inclusion of processes
  - Coupling
- Compare to other uncertainties
  - Stochastic fracture network
  - Uncertain inputs
  - Conceptual uncertainties

D-23 Task F1 Crystalline

Section Heading	Test Cases	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







FEATURES

Geologic setting

Complexity of model domain (check one).

- ☐ Our meshing software can handle an island with simple shoreline and topography.
  - o Input format for irregular surfaces or volumes is ________________.
- ☐ Our meshing software is better suited to a rectilinear (box-shaped) model domain.

Emplacement concept

[Question raised at kick-off meeting: Is it desirable to simplify the model domain by choosing an emplacement concept that uses in-drift axial emplacement?]
Preferred choice is (check one):

- ☐ KBS-3V (4-PWR canister in vertical deposition hole)
- ☐ KBS-3H (4-PWR canister in horizontal boreholes)
- ☐ In-drift axial emplacement of 4-PWR canisters
- ☐ In-drift axial emplacement of larger (12-PWR) canisters
- ☐ Other (please describe): ___________

Inventory

How much waste (check one):

- ☐ Proposed inventory sounds good: 4350 MTU (2500 4-PWR canisters)
- ☐ <4350 MTU (please suggest): _____________
- ☐ >4350 MTU (please be aware of simulation size): _____________

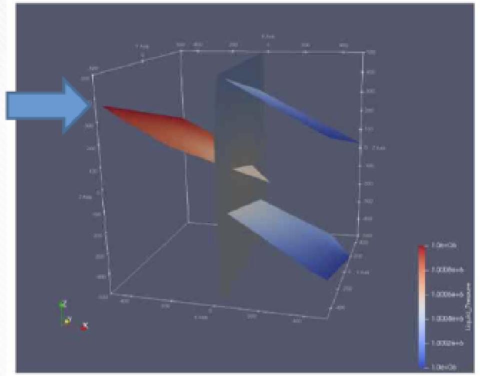
Waste characteristics (check all that apply)

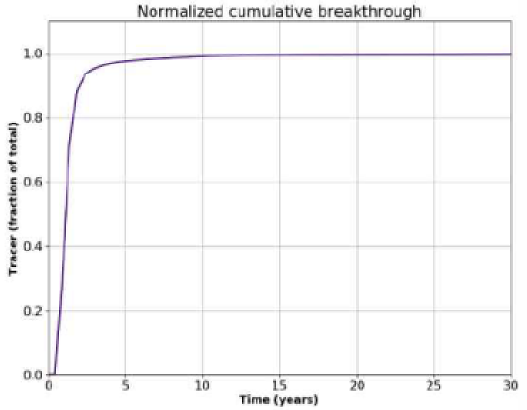
- ☐ Pressurized water reactor (PWR) spent nuclear fuel assemblies with radionuclide inventory and heat of decay calculated assuming initial enrichment of 4.73 wt% U-235, 60 GWd/MTU burnup, 50 years out of reactor (OoR) (Carter et al. 2013) – to be provided by U.S. team.
- ☐ Instead of this (please describe): ______________
- ☐ In addition to this (please describe): _____________

Fractured Rock Transport Benchmarks

- 4-Fracture – Deterministic fractures

Particle injection

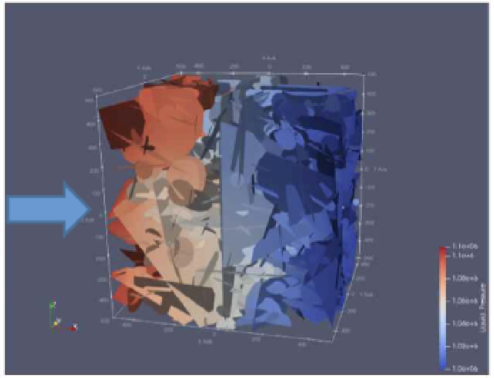


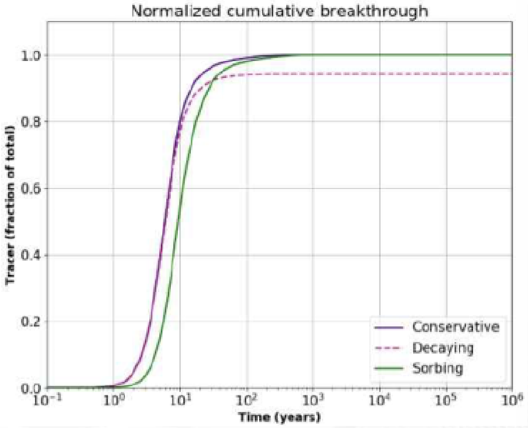


- Simulation time
  - 30 years

- 4-Fracture+ – Stochastic fractures

Particle injection



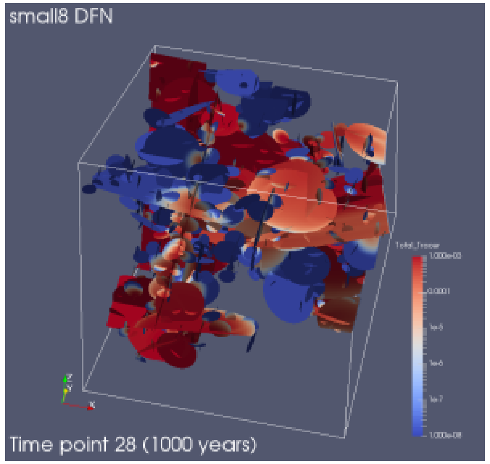


- Simulation time
  - 1x10^6 years
- Cases
  - Conservative
  - Decaying
  - Sorbing

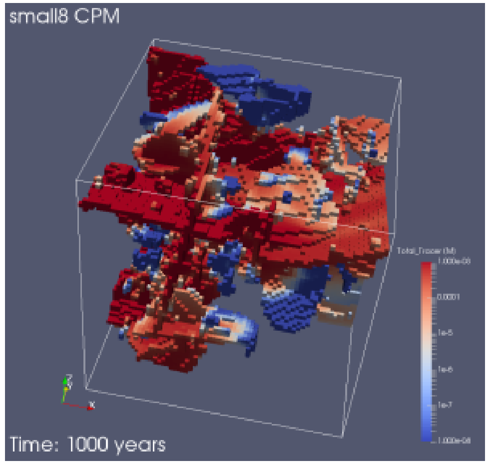
KAERI Korea Atomic Energy Research Institute

4

Lee et al. Task F1 presentation



vs.



vs. other?

Benchmark Results From …

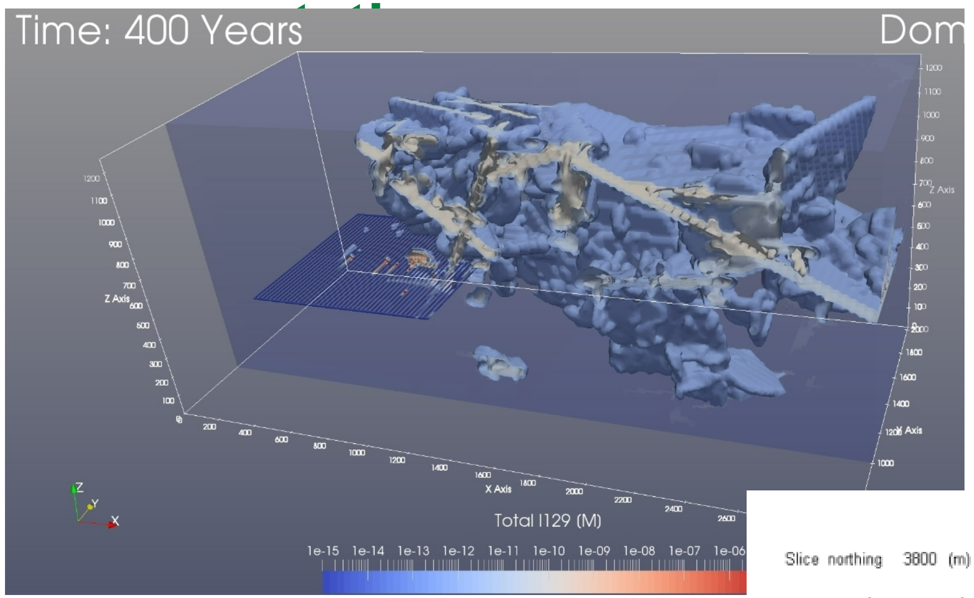
Team	Modeling Tool	Modeling Approach
BGR	FracMan/OpenGeoSys	• DFN + ECPM, mesh conforming to deterministic fractures, w/ ADE
CNSC	COMSOL	• DFN (4-frac) w/ ADE • DFN + ECPM (4-frac+) w/ ADE
DOE (SNL/LANL)	dfnWorks/PFLOTRAN	• DFN w/ particle tracking or ADE • ECPM (2 methods) w/ ADE
TaiPower (INER)	DarcyTools	• ECPM w/ particle tracking
KAERI	COMSOL (Darcy's Law Module, Transport of Diluted Species in Porous Media Module)	• DFN w/ ADE • ECPM (2 methods) w/ ADE
NWMO	COMSOL (Fracture Flow Module, Transport of Diluted Species in Fractures Module)	• DFN w/ ADE
SURAO	dfnWorks/PFLOTRAN	• ECPM (2 methods) w/ ADE

DFN discrete fracture network
ADE advection dispersion equation
ECPM equivalent continuous porous medium

And then there are the teams whose approach to PA makes these benchmarks irrelevant!

Modeling Approach?

Various approaches to achieve desired computational efficiency and adequate



3-D ECPM

Mariner et al. 2016

3-D CPM w/ deterministic features

NWMO TR-2012-16

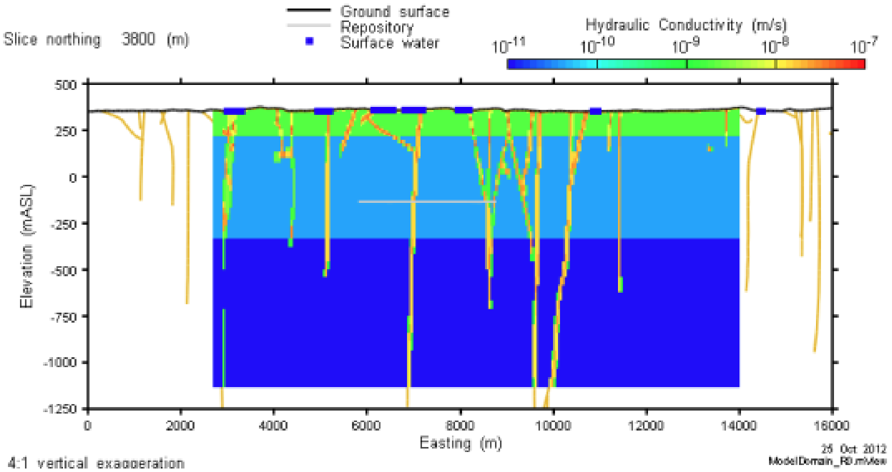
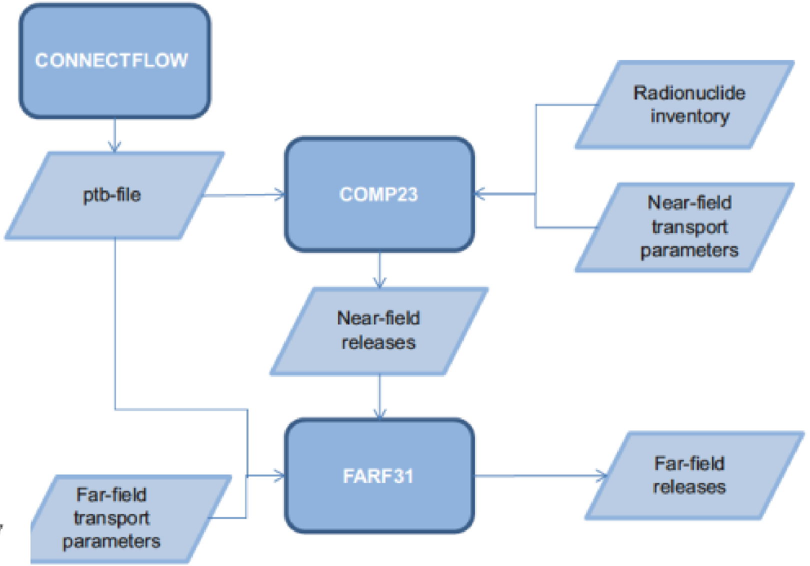


Figure 7-9: Sub-Regional Model: EPM Fracture Network and Vertical Hydraulic Conductivity Profile



ure 3-2. Model linkages and data flows for radionuclide transport simulations using FARF31.

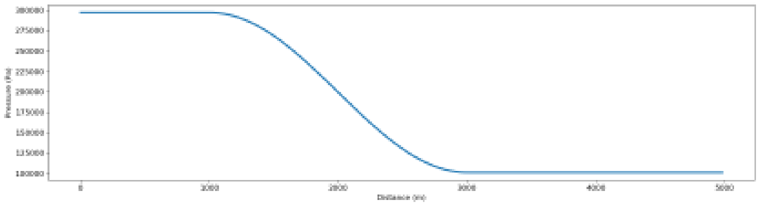
1-D flow paths abstracted from D

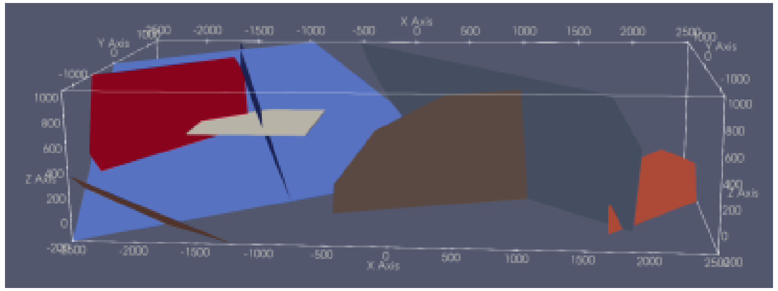
SKB TR-10-50

ECPM equivalent continuous porous medium
CPM continuous porous medium
DFN discrete fracture network

Lessons Learned and Next Steps

- Benchmarks
  - For some teams, the stochastic fractures benchmark is not relevant, because they won't resolve this level of heterogeneity in their PA simulations.
  - For other teams, working to reduce the discrepancies in the benchmark results will help them refine their modeling approaches.
- Designing a reference case fit for purpose is tricky
  - Amenable to a variety of modeling approaches
  - Simple enough that we understand what we're comparing
  - Rich enough that different teams will make different choices
- Next steps
  - Finish up fractured rock transport benchmarks
  - Convene a small team to pin down initial reference case
  - Start reference case simulations around time of Fall Workshop



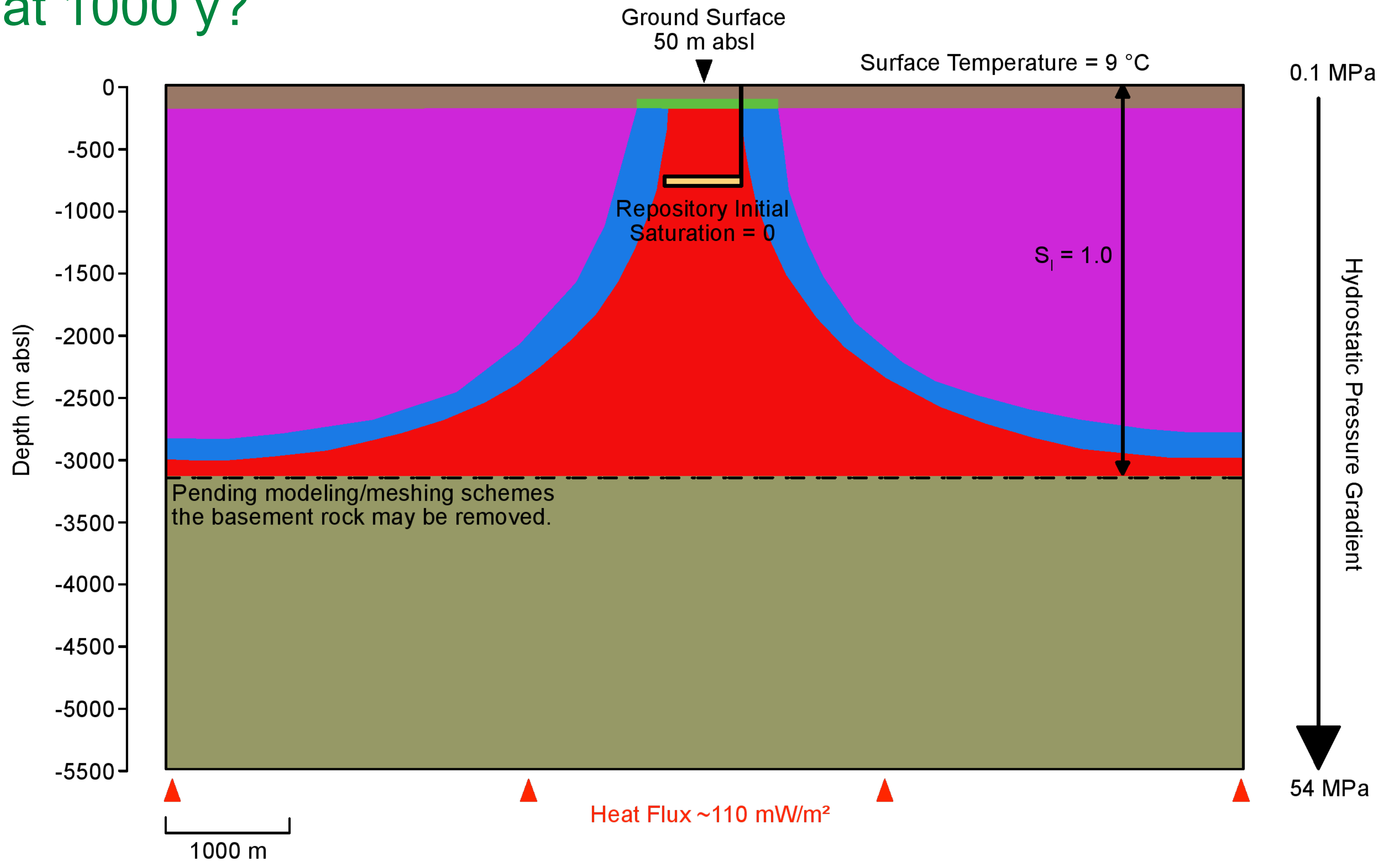


"What if *xx* waste packages fail at 10k years?"

D-23 Task F2 Salt

What if the shaft seals fail at 1000 y?

- 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)



Modeling Approach

Team	Modeling Tool	Modeling Approach
COVRA	COMSOL	• Detailed representation of repository • Neglect impermeable host rock?
DOE (SNL/LANL)	PFLOTRAN	• Hex or Voronoi mesh? • Include all volumes/materials
GRS	LOPOS, then later NaTREND	• "Looped structures in repositories" • Segmented model

Lessons Learned and Next Steps

- Designing a reference case has been relatively easy
  - This activity was clearly stated to be the first goal of the project
  - Smaller number of teams
  - Many participants had previously worked together
- Next steps
  - 1-D and 2-D transport benchmarks
  - Fill in last few details of the reference case
  - Preliminary reference case simulations for Fall Workshop

DECOVALEX Task E

Brine Availability Test in Salt

Task E Goals

- Understand and predict THMC processes impacting *brine availability* in salt

1. Single-phase unheated brine inflow
2. Heat conduction during BATS heater test
3. Analytical solution for thermal pressurization
4. Two-phase flow in BATS drift
5. Brine production pulse after turning off heaters

- WIPP Test Cases:
  - Small-Scale Brine Inflow test (1987-1992)
  - McTigue (1986, 1990) analytical solution
  - Ongoing heated Brine Availability Test in Salt (BATS)

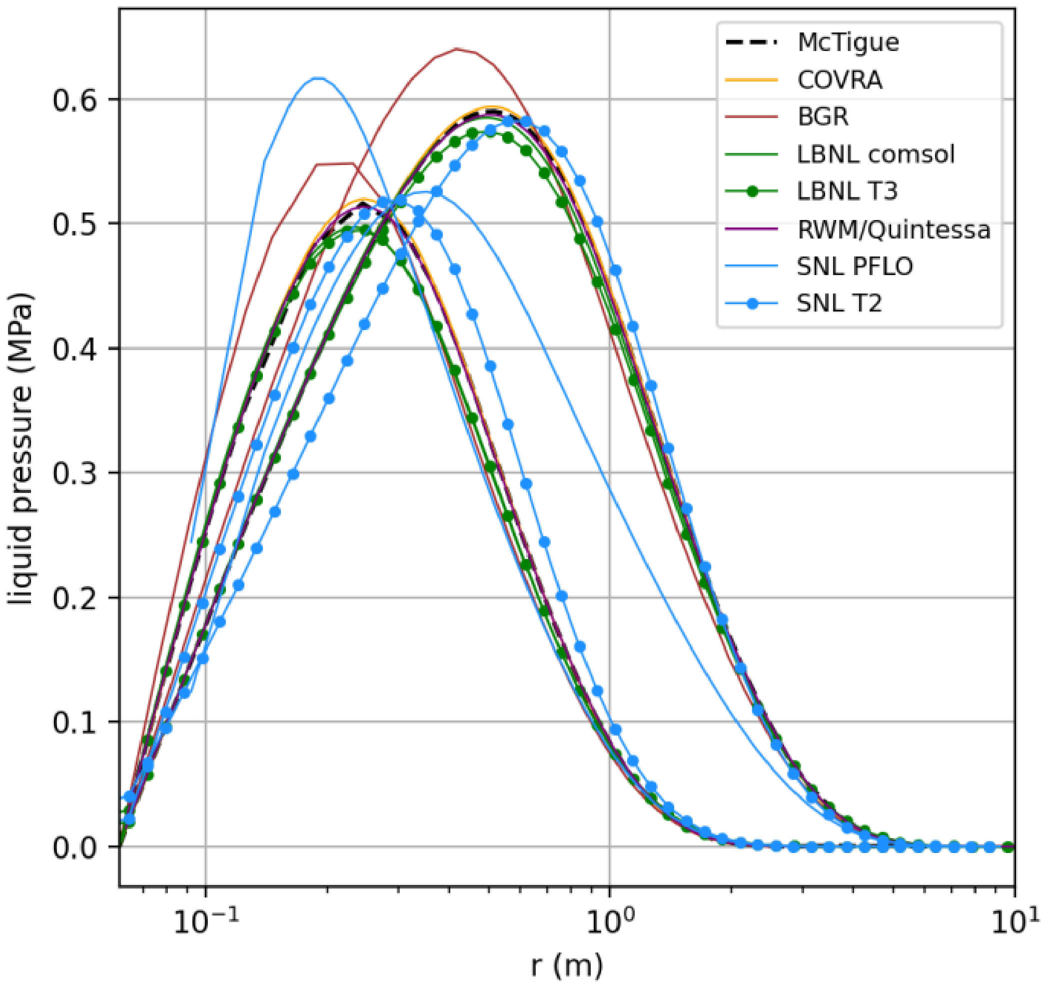
Task E Participating Teams

Team	Modeling Tool	Type
BGR	OpenGeoSys V5	FE multiphysics
COVRA	COMSOL	FE multiphysics
GRS	CODE_BRIGHT	FE THMC
DOE: LANL/LBNL/SNL	COMSOL / FEHM / TOUGH -FLAC / PFLOTRAN	FE Multiphysics & FV TH(M)C
RWM/Quintessa	QPAC	FV multiphysics

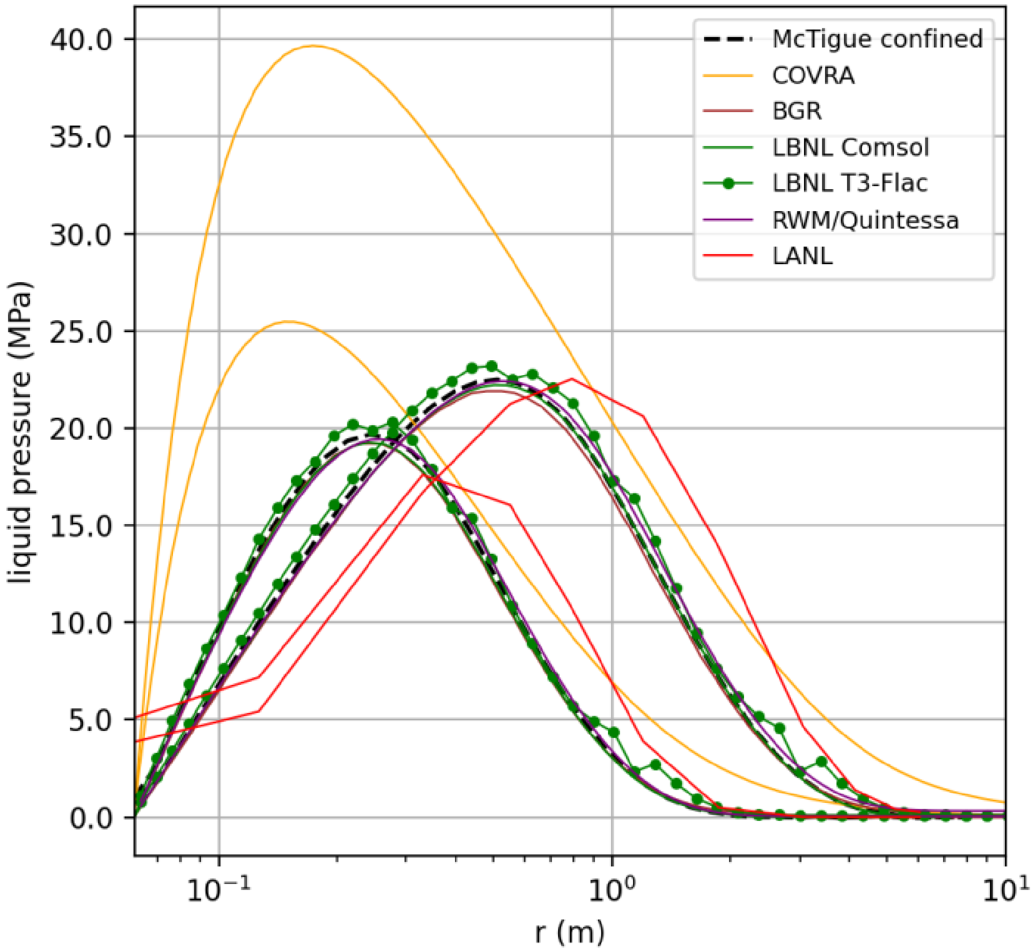
FE: finite element, FV: finite volume (integrated finite differences)

Task E Step 1a Comparison – Thermal Pressurization

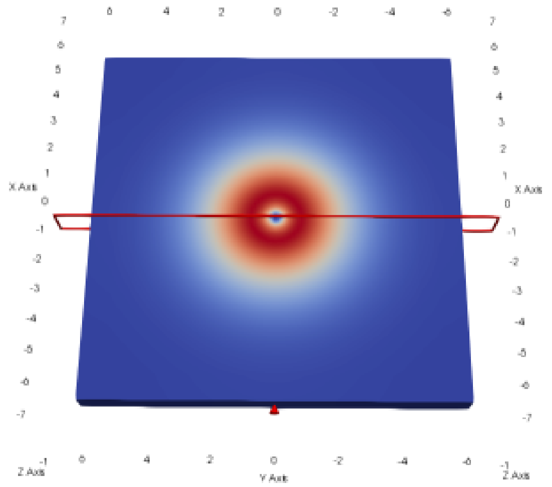
TH Response



THM Response



Task E Step 1a Lessons Learned



- Thermal pressurization response
  - "Unconfined" TH response
    - Fluid thermal expansion only
    - THM response with 40x thermal expansion & modified compressibility
  - Confined THM response
    - Fluid & solid thermal expansion, pushing against regional confinement
- "Dam" of high pressure liquid, reduces inflow during heating
  - How will partial saturation and two-phase flow impact this?

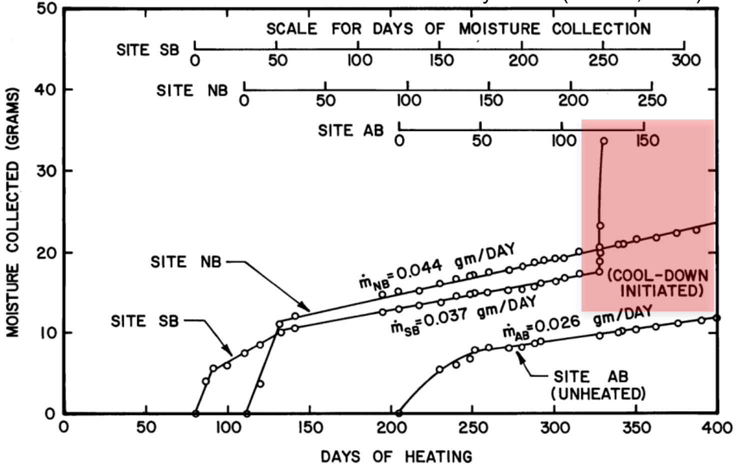
- Comparing models against analytical solution can be complex

Task E Step 2 – Starting Soon

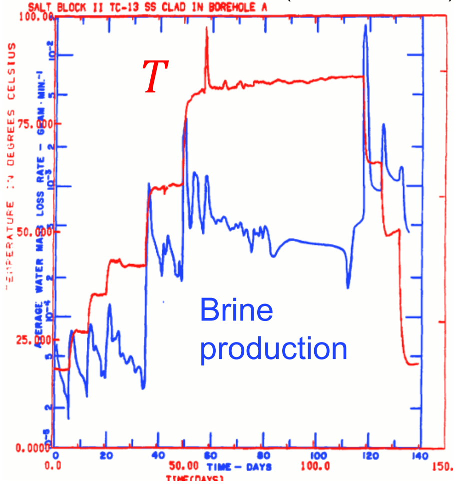
2. TH²M heated brine inflow test case

a) Predict brine production during increases and decreases in *T*

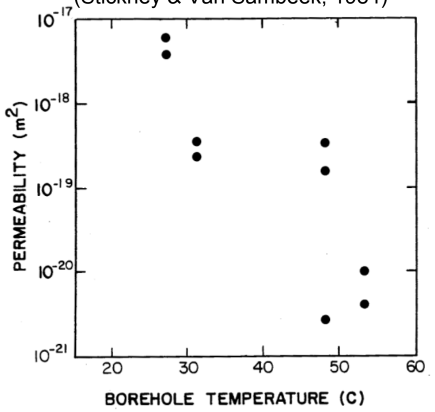
Avery Island (Krause, 1983)

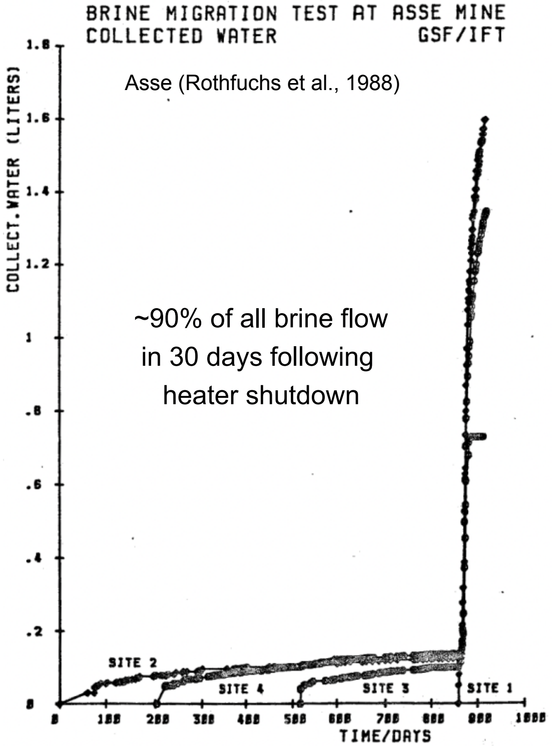


1-m bedded salt lab test (Hohlfelder, 1979)



Avery Island permeability data (Stickney & Van Sambeek, 1984)





- Permeability as a function of stress, due to thermal expansion?
- Permeability as a function of temperature?
- Something else?

Task E Conclusions

- Thermal Pressurization analytical solution was a big learning experience
  - TH vs. THM (confined vs. unconfined)
  - *Huge* difference in pressure from thermal pressurization
- Slowed down planned jump to two-phase flow
  - Two-phase flow models are big jump up in complexity
  - Delaying start to better understand thermal pressurization more
  - Building understanding of complex problems takes time
- Each team brings something unique and different to Task E
  - Different numerical tools
  - Different team member backgrounds
  - Different eye for what is important