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Spent Fuel and Waste Science and Technology (SFWST)

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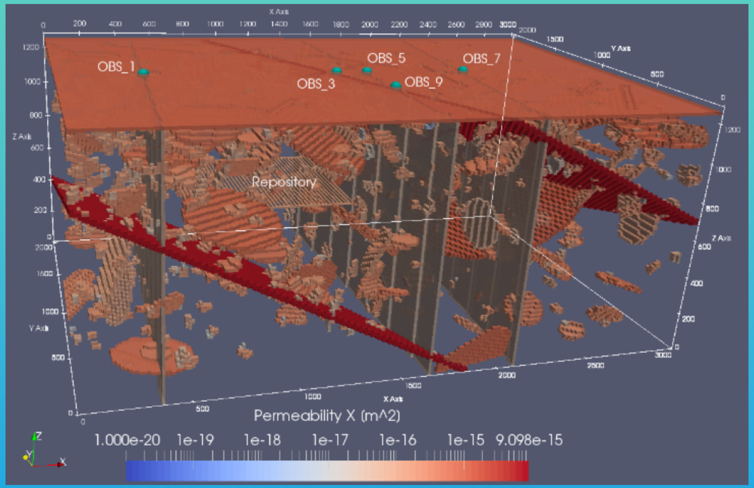


# Reference Case Simulation

Nuclear Waste Technical Review Board

Fact-finding meeting

October 13-14, 2021

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Sandia National Laboratories

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# Post-closure Safety Assessment

## 1. Introduction, Purpose, and Context

## 2. Safety Strategy

### 2.1 Management Strategy
a. Organizational/mgmt. structure
b. Safety culture & QA
c. Planning and Work Control
d. Knowledge management
e. Oversight groups

### 2.2 Siting & Design Strategy
a. National laws
b. Site selection basis & robustness
c. Design requirements
d. Disposal concepts
e. Intergenerational equity

### 2.3 Assessment Strategy
a. Regulations and rules
b. Performance goals/safety criteria
c. Safety functions/multiple barriers
d. Uncertainty characterization
e. RD&D prioritization guidance

## 3. Technical Bases

### 3.1 Site Selection
a. Siting methodology
b. Repository concept selection
c. FEPs Identification
d. Technology development
e. Transportation considerations
f. Integration with storage facilities

### 3.2 Pre-closure Basis
a. Repository design & layout
b. Waste package design
c. Construction requirements & schedule
d. Operations & surface facility
e. Waste acceptance criteria
f. Impact of pre-closure activities on post-closure

### 3.3 Post-closure Bases (FEPs)

#### 3.3.1 Waste & Engineered Barriers Technical Basis
a. Inventory characterization
b. WF/WP technical basis
c. Buffer/backfill technical basis
d. Shafts/seals technical basis
e. UQ (aleatory, epistemic)

#### 3.3.2 Geosphere/ Natural Barriers Technical Basis
a. Site characterization
b. Host rock/DRZ technical basis
c. Aquifer/other geologic units technical basis
d. UQ (aleatory, epistemic)

#### 3.3.3 Biosphere Technical Basis
a. Biosphere & surface environment:
- Surface environment
- Flora & fauna
- Human behavior

## 4. Disposal System Safety Evaluation

### 4.1 Pre-closure Safety Analysis
a. Surface facilities and packaging
b. Mining and drilling
c. Underground transfer and handling
d. Emplacement operations
e. Design basis events & probabilities
f. Pre-closure model/software validation
g. Criticality analyses
h. Dose/consequence analyses

### 4.2 Post-closure Safety Assessment
a. FEPs analysis/screening
b. Scenario construction/screening
c. PA model/software validation
d. Barrier/safety function analyses and subsystem analyses
e. PA and Process Model Analyses/Results
f. Uncertainty characterization and analysis
g. Sensitivity analyses

### 4.3 Confidence Enhancement
a. R&D prioritization
b. Natural/anthropogenic analogues
c. URL & large-scale demonstrations
d. Monitoring and performance confirmation
e. International consensus & peer review
f. Verification, validation, transparency
g. Qualitative and robustness arguments

## 5. Synthesis & Conclusions
a. Key findings and statement(s) of confidence
b. Discussion/disposition of remaining uncertainties
c. Path forward

Sevougian et al. 2019b

# Generic Features, Events, and Processes (FEPs)

**Source (Inventory and Waste Form)**
- Radionuclide inventory (heat generation, decay and ingrowth)
- Waste form degradation (dissolution processes)
- Gas generation
- Radionuclide release and transport (mobilization, early release [e.g., from gap and grain boundaries], precipitation/dissolution)

**Near Field (Waste Package, Buffer, Backfill, Seals/Liner, and Disturbed Rock Zone (DRZ))**
- Waste package degradation (corrosion processes, mechanical damage, early failures)
- Evolution/degradation of engineered barrier system (EBS) components and DRZ
- Effects from rockfall, drift collapse (e.g., salt creep)
- Fluid flow and radionuclide transport (advection, dispersion, diffusion, sorption, decay and ingrowth)
- Chemical interactions (aqueous speciation, mineral precipitation/dissolution, reaction with degraded materials, surface complexation, radiolysis)
- Thermal effects on flow and chemistry
- Effects from disruptive events (seismicity, human intrusion)

**Far Field (Host Rock and Other Units)**
- Fluid flow and radionuclide transport (advection, dispersion, diffusion, sorption, decay and ingrowth)
- Effects of fracture flow (e.g., dual porosity/permeability, discrete fracture)
- Groundwater chemistry

**Receptor (Biosphere)**
- Dilution due to mixing of contaminated and uncontaminated waters
- Receptor characteristics (basis for converting radionuclide concentrations in groundwater to dose)

**Key**

Red = FEP included, at least to some degree

Black = FEP capability lacking or excluded so far

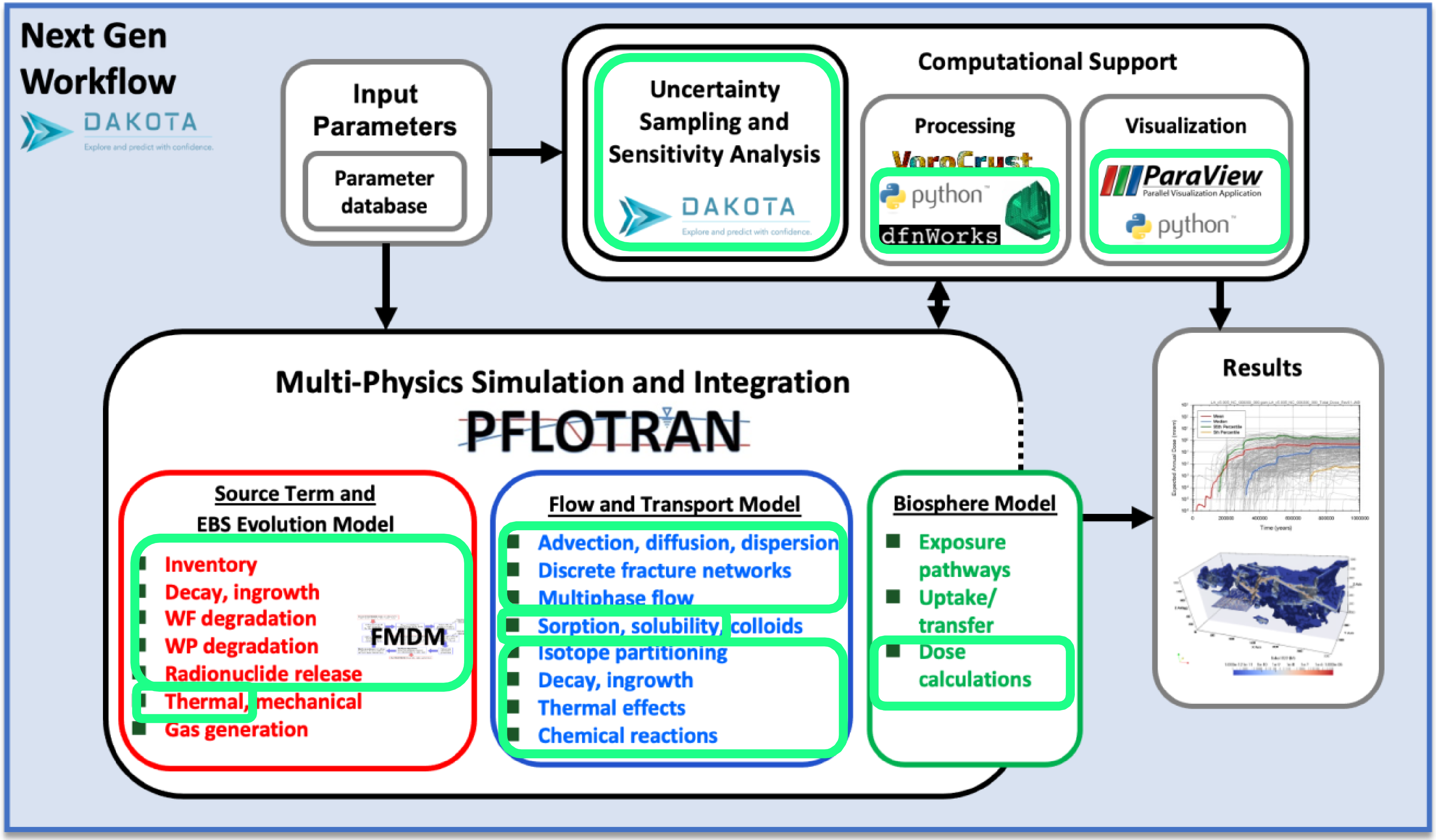
- Chemical, mechanical, and disruptive features, events, and processes (FEPs) account for many of the excluded (or yet-to-be-implemented) FEPs

# 2019 Roadmap Update – High Impact R&D Topics

- **High-temperature impacts**
- Buffer and seal studies
- Coupled processes in salt
- Gas flow in the engineered barrier system
- **Criticality**
- **Waste package degradation**
- In-package chemistry
- **Generic performance assessment models**
- **Radionuclide transport**

Sevougian et al. 201

# GDSA Framework



# Reference case simulations overview

- Overarching goal: Develop and demonstrate simulation and analysis capability to provide a sound technical basis for multiple viable disposal options
  - Conduct studies on potential host rocks
  - Find gaps and enhance capability in process models, workflow, etc
  - Drive development of process models
  - Focusing on high-temperature waste package disposal in recent years
- In all cases
  - Only undisturbed scenarios
  - Generic FEPs screening (Vaughn, 2012)
  - Uncertainty and sensitivity analysis using DAKOTA
  - Main performance metric is peak iodine in aquifer

# Reference case simulation overview – generic concepts and inventories

| | | Defense SNF & HLW | CSNF 4-PWR | CSNF 12-PWR | CSNF 21-PWR | CSNF 24- & 37-PWR |
|---|---|---|---|---|---|---|
| **Shale** | $\kappa$ = 1.2 W/(m-K) | Stein et al. 2017 Simulation | Mariner et al. 2017 Simulation | Mariner et al. 2017 Simulation | Stein et al. 2020 Concept | Sevougian et al. 2019 Simulation |
| | Waste Package Heat Source<br>Max Temperature | ≤ 1 kW<br>100° C | 1 kW<br>105° C | 3 kW<br>150° C | 4 kW<br>250° C | 4 & 6 kW<br>175° & 180° |
| **Crystalline** | $\kappa$ = 2.5 W/(m-K) | Sevougian et al. 2016 Simulation | DECOVALEX-2023 Concept | Swiler et al. 2021 Simulation | – | – |
| | Waste Package Heat Source<br>Max Temperature | ≤ 1 kW<br>85° C | 1 kW<br>100° C | 3 kW<br>130° C | | |
| **Salt** | $\kappa$ = 4.9 W/(m-K) | Sevougian et al. 2016 Simulation | – | Mariner et al. 2015 Simulation | SNL 2019 Concept | LaForce et al. 2020 Simulation |
| | Waste Package Heat Source<br>Max Temperature | ≤ 1 kW<br>90° C | | 6 kW<br>150° C | 10 kW<br>200° C | 7 & 9 kW<br>120° & 150° |

$\kappa$ = thermal conductivity (of the liquid-saturated host rock)

SNF = spent nuclear fuel

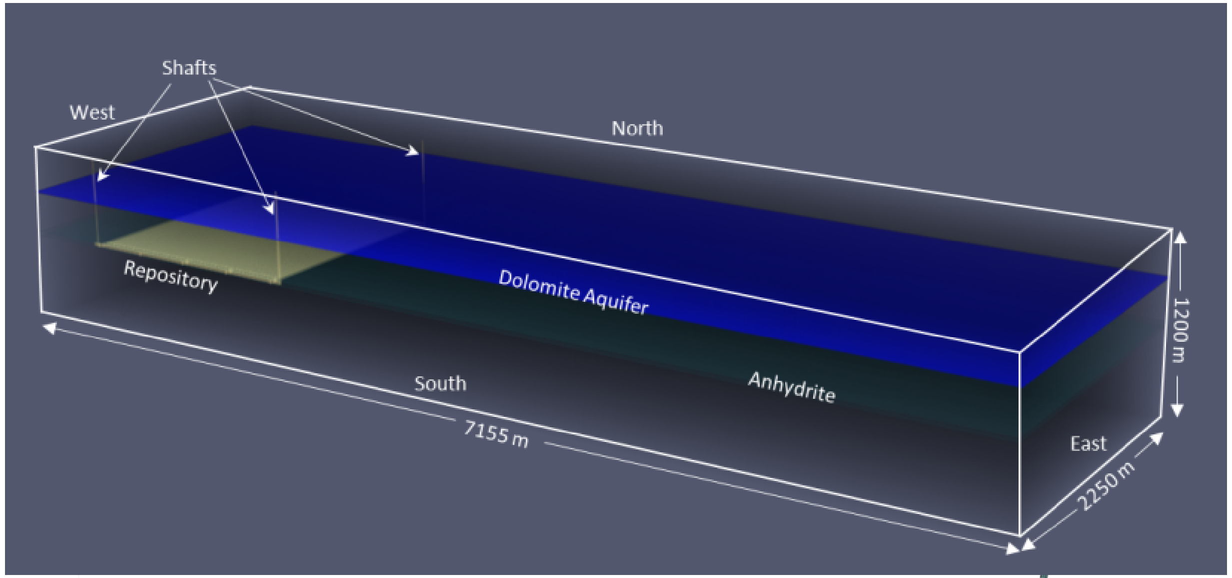
HLW = high level waste

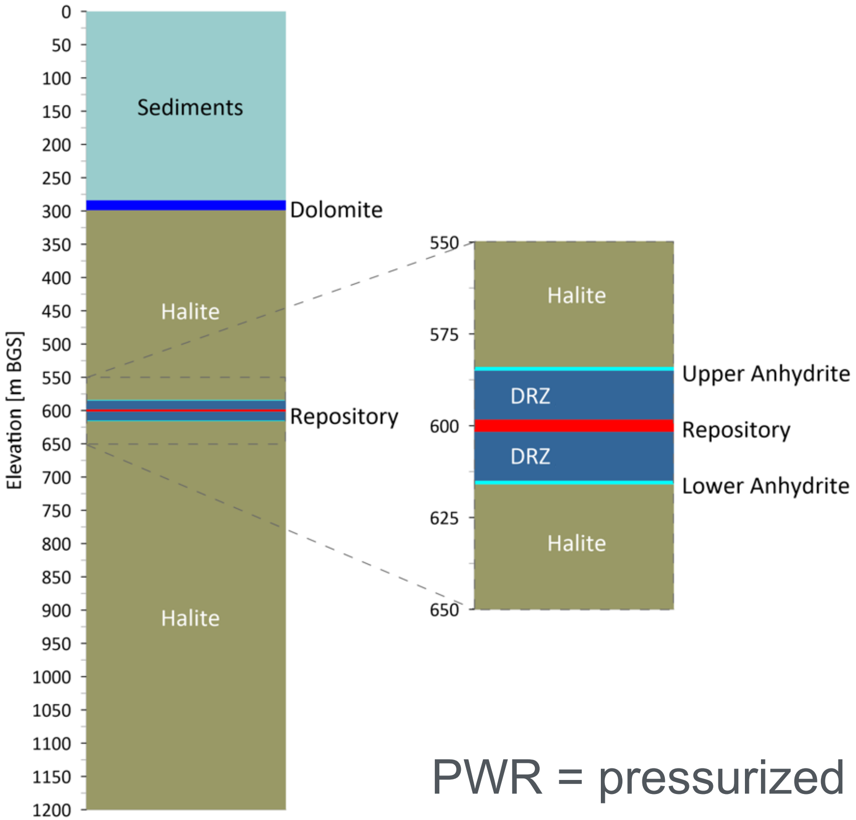
CSNF = commercial spent nuclear fuel

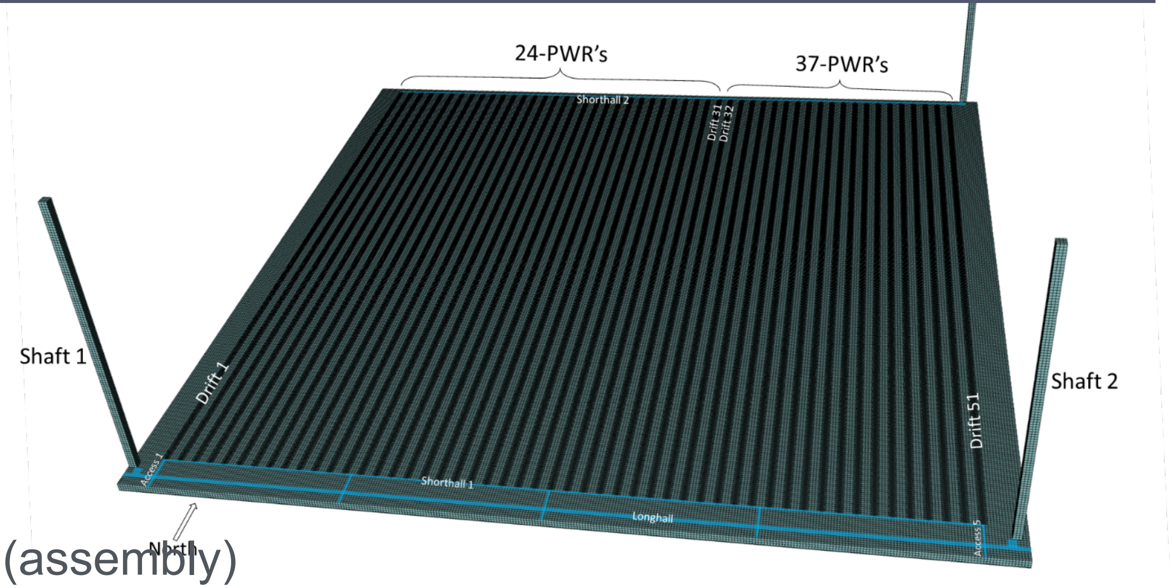
PWR = pressurized water reactor (assembly); represents waste package capacity

# Salt reference case (LaForce et al, 2020)

- 3100 24-PWR and 2000 37-PWR waste packages in 102 drifts (half-symmetry domain)
- 200 probabilistic simulations



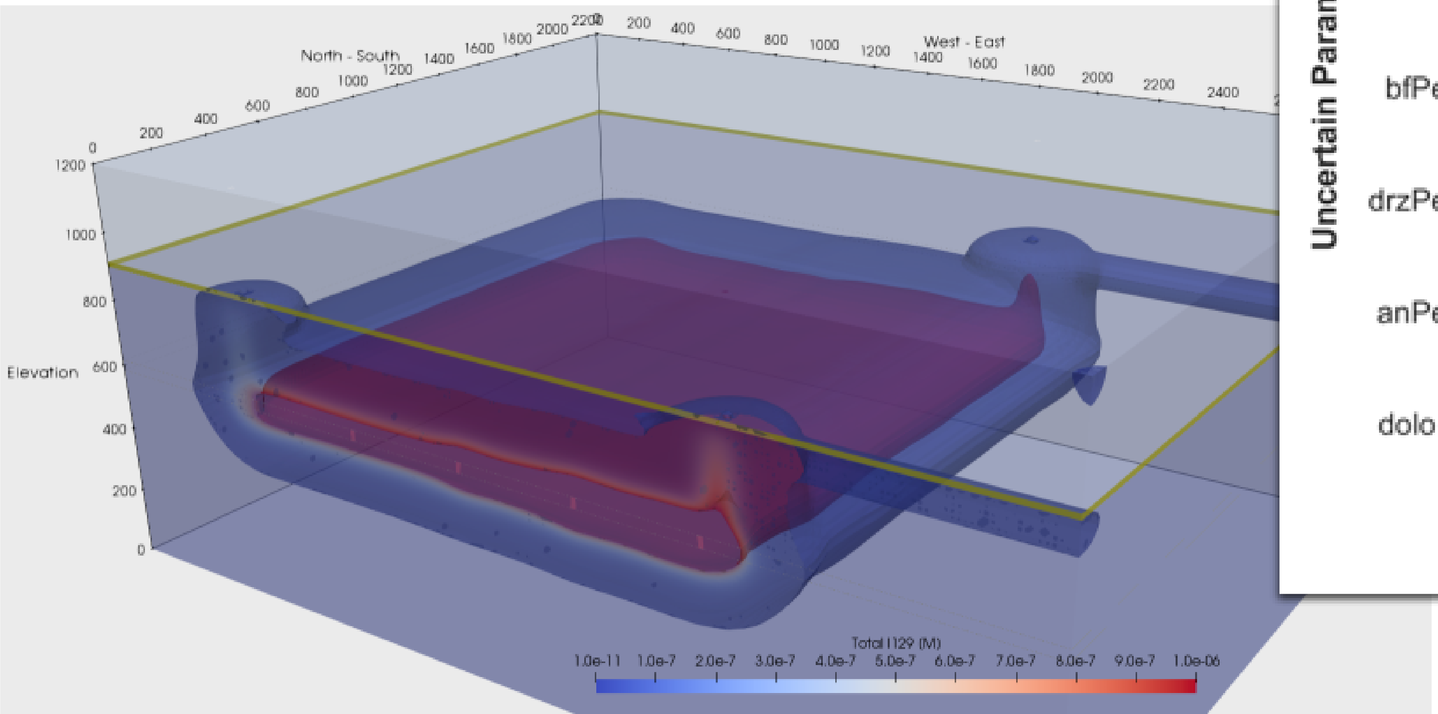



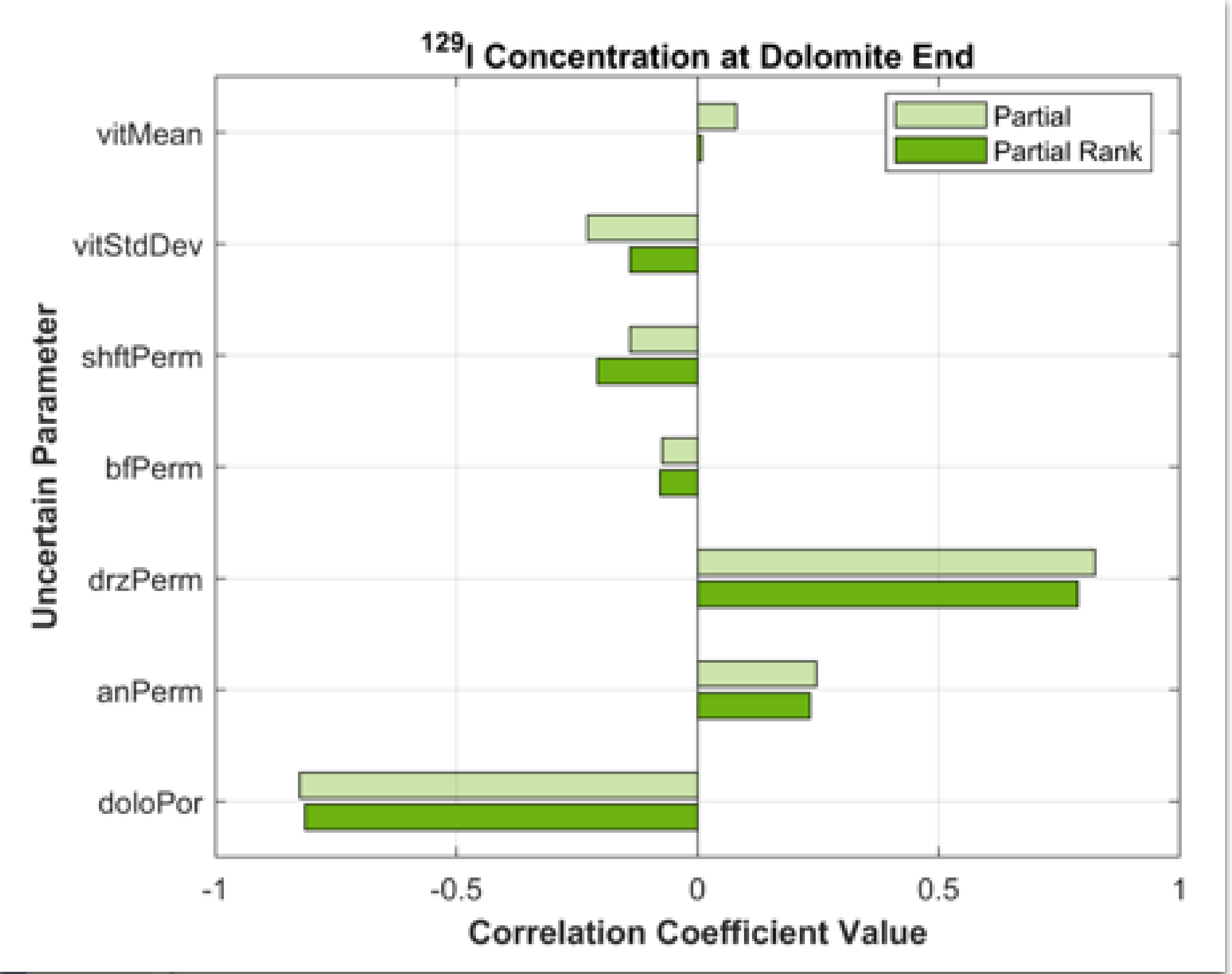

PWR = pressurized water reactor (assembly)

# Salt reference case results (LaForce et al, 2020)

- Partial-correlation coefficient values
- Peak I-129 concentration is sensitive to
  - DRZ permeability
  - Dolomite porosity/permeability

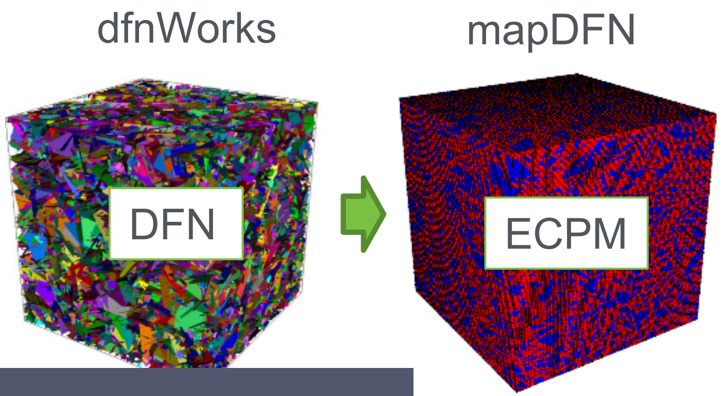



$^{129}$I concentration after 1,000,000 years ($10^{-11}$ to $10^{-6}$ M shown)

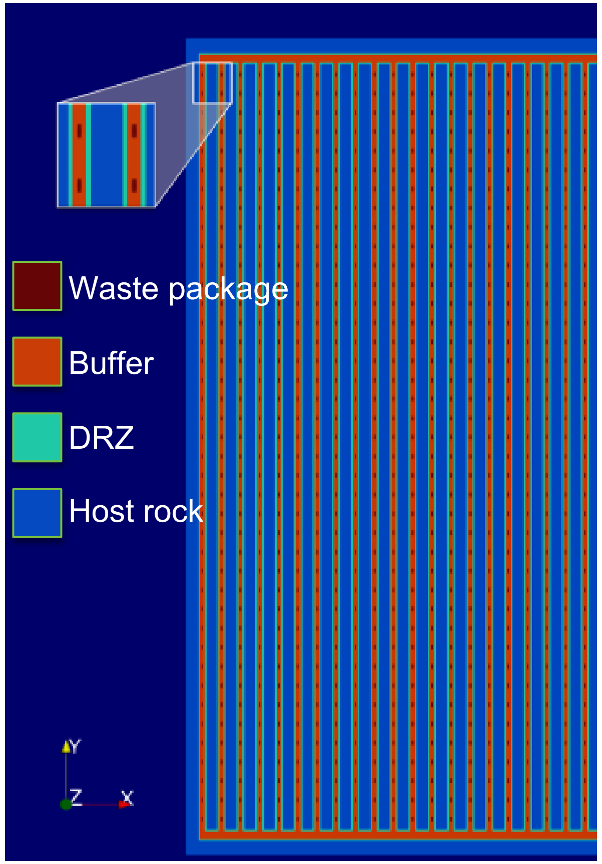


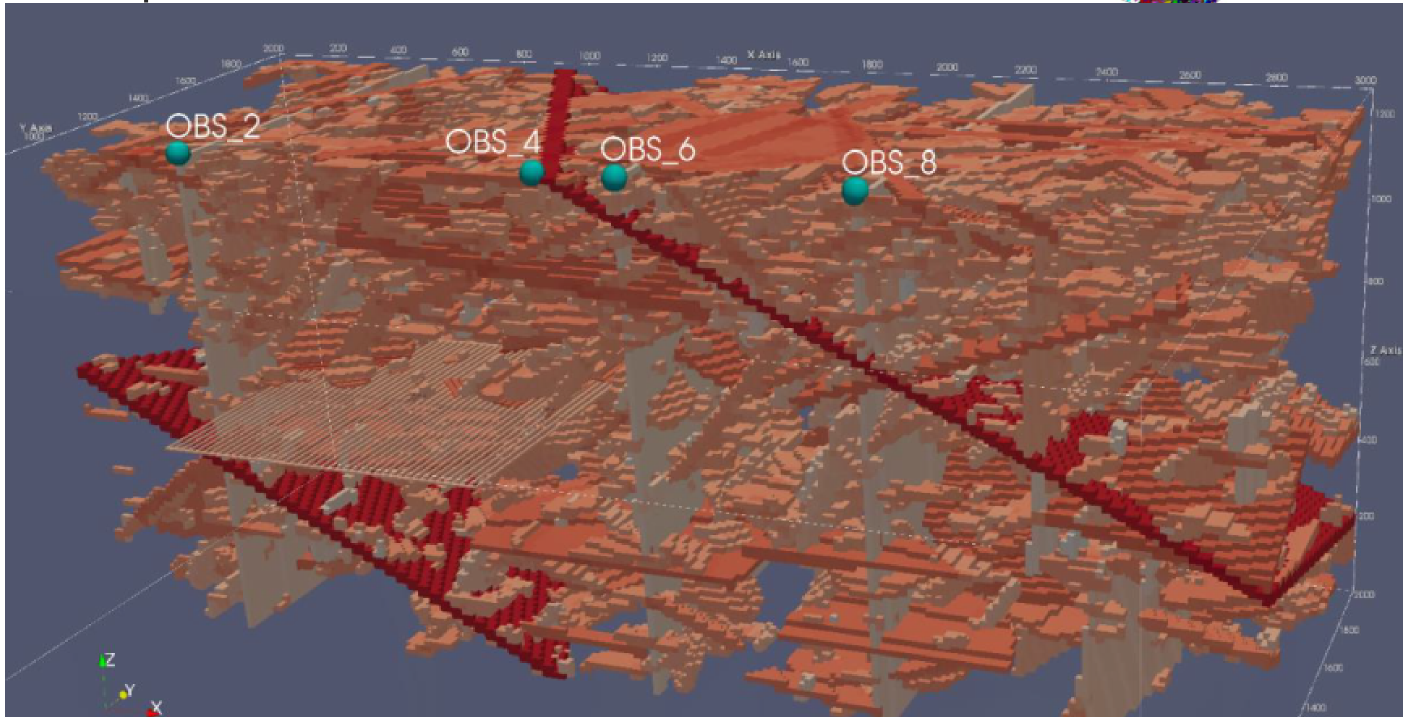
# Crystalline reference case (Swiler et al. 2021)

- 1000 realizations
- Discrete fracture networks (DFNs)
- Deterministic and stochastic fracture zones (25 realizations)
- 1680 12-PWR waste packages in 42 disposal drifts




Map view of half of the repository colored by material type

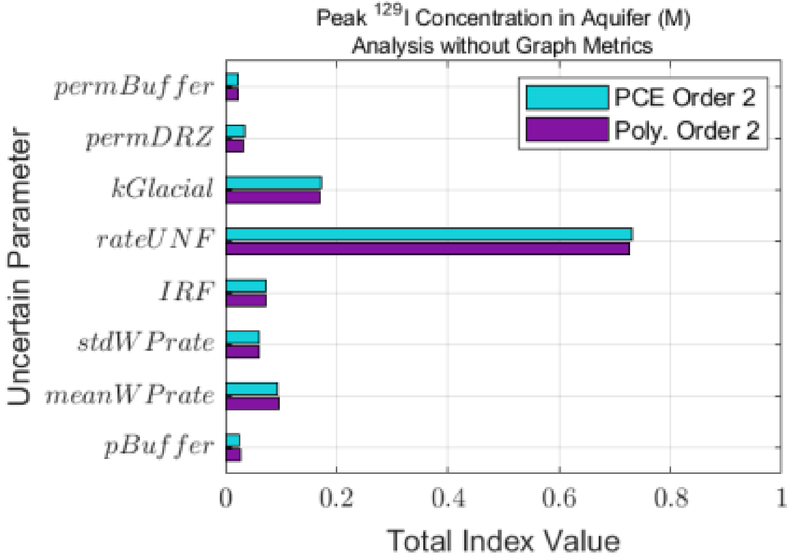


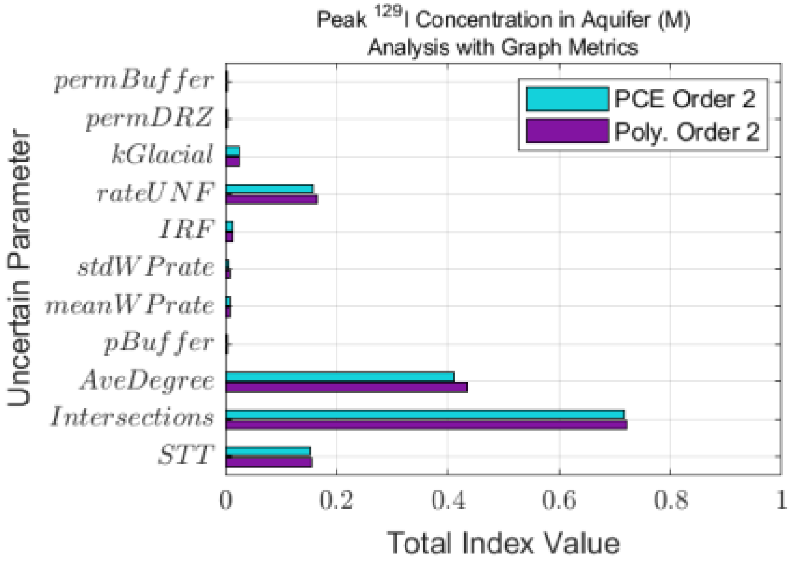




Cut-away of a DFN realization mapped to the equivalent continuous porous medium (ECPM), showing the full repository and the far half of the model domain.

# Crystalline reference case results

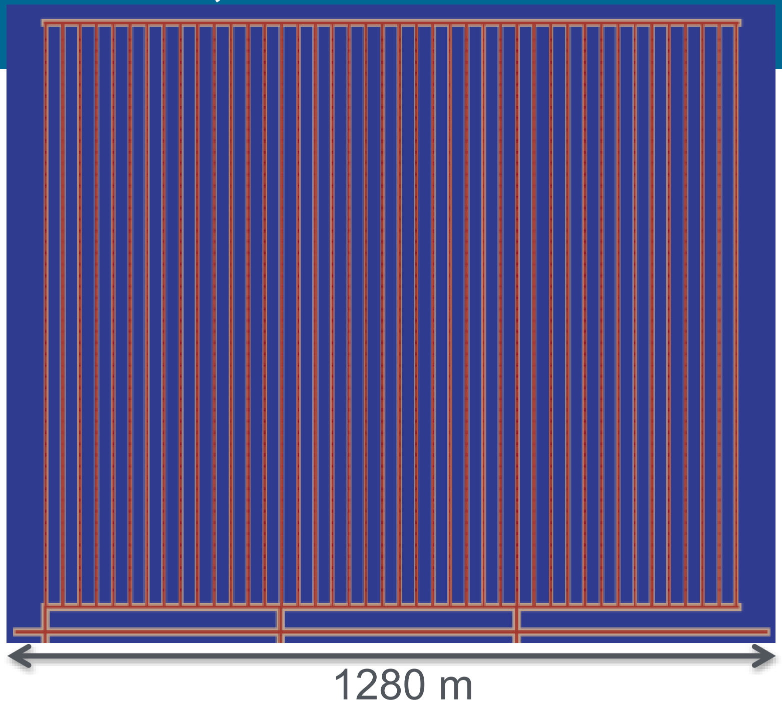
- Total sensitivity indices
- When stochastic variation in the fracture network is not considered in the sensitivity analysis:
  - Peak I-129 concentration appears most sensitive to the rate of spent nuclear fuel dissolution
- When stochastic variation in the fracture network is considered in sensitivity analysis:
  - A stronger dependence on characteristics of the fracture network is apparent

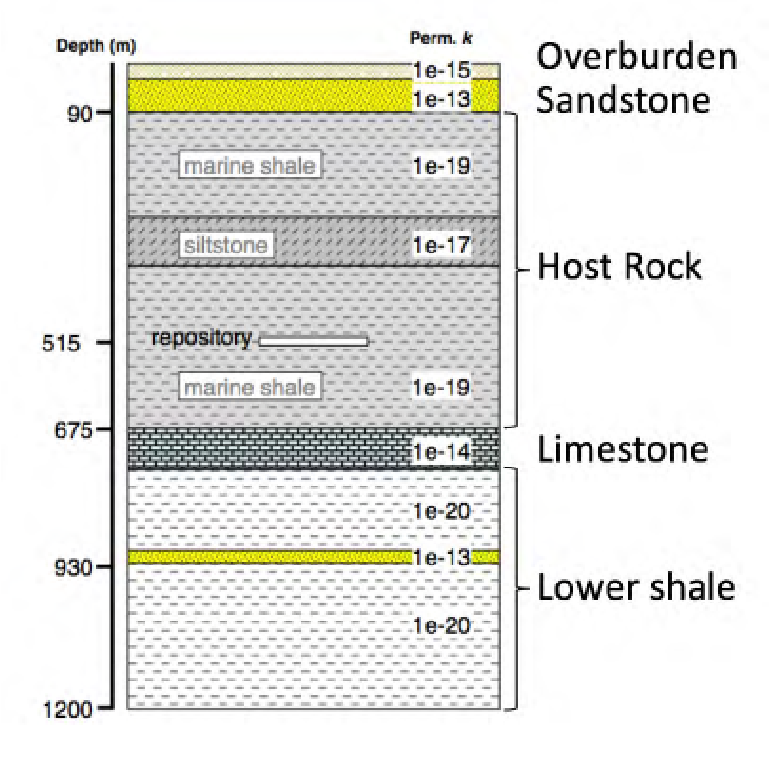


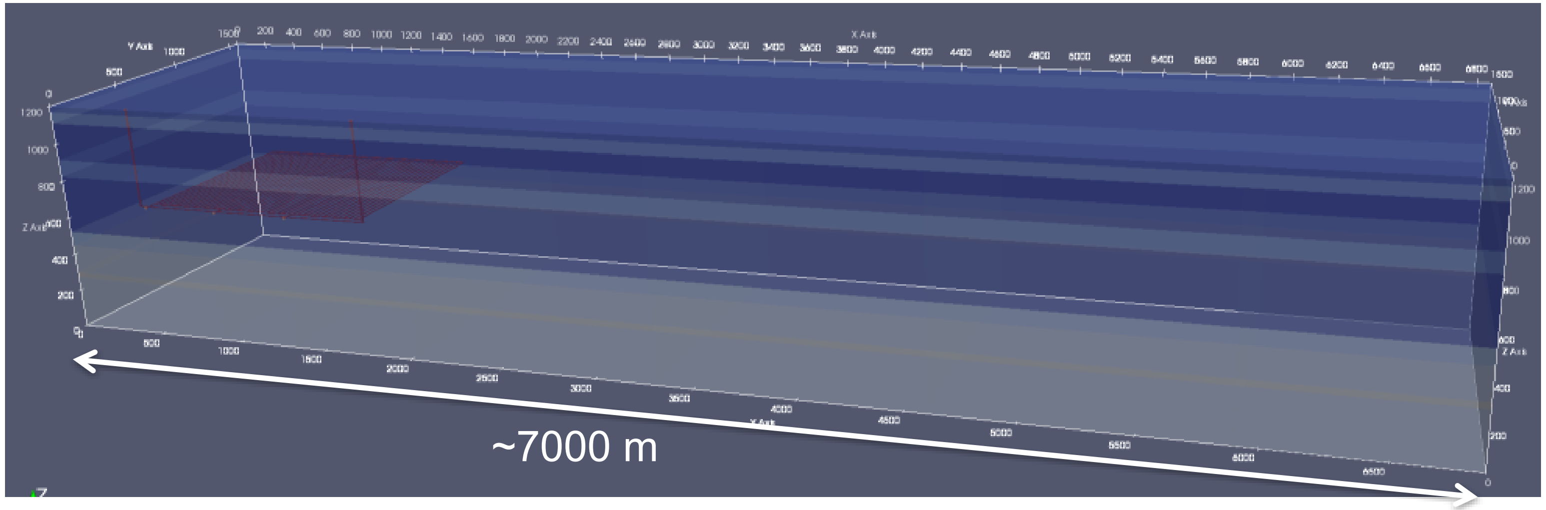



# Shale (argillite) reference case (Mariner et al. 2017; Swiler et al. 2019)

- 4200 12-PWR waste packages in 84 drifts (half-symmetry domain)
- Incremental Latin hypercube sampling (50, 100, 200 samples)

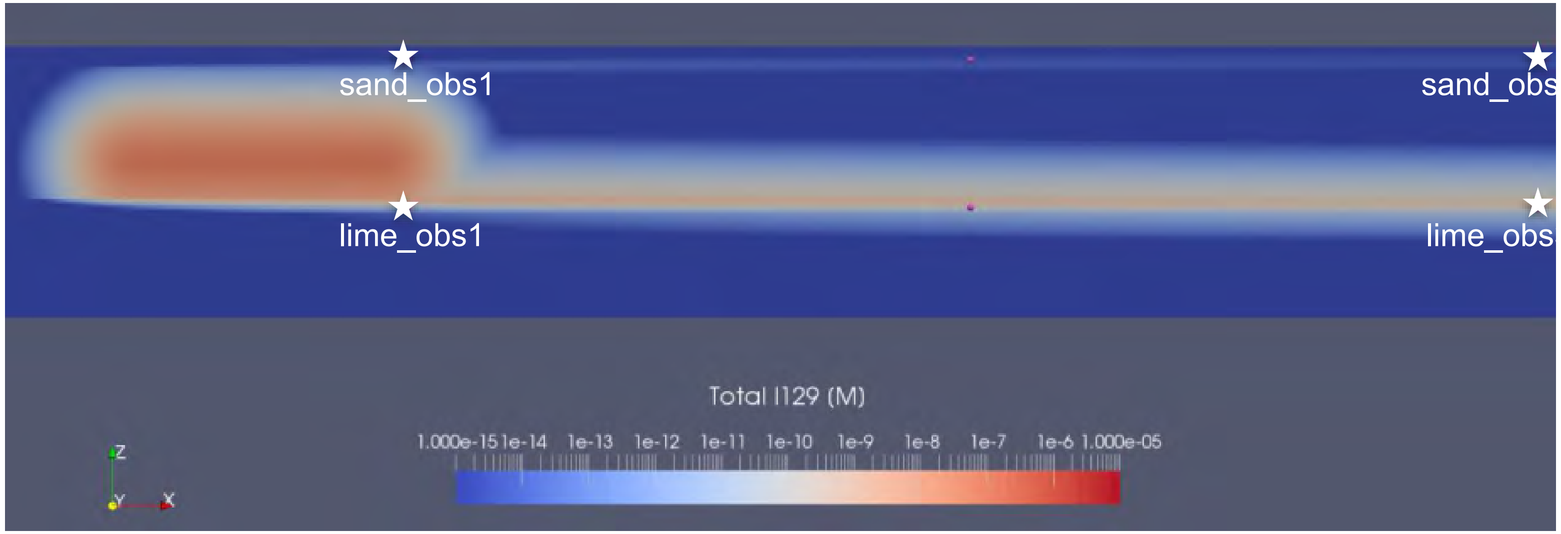


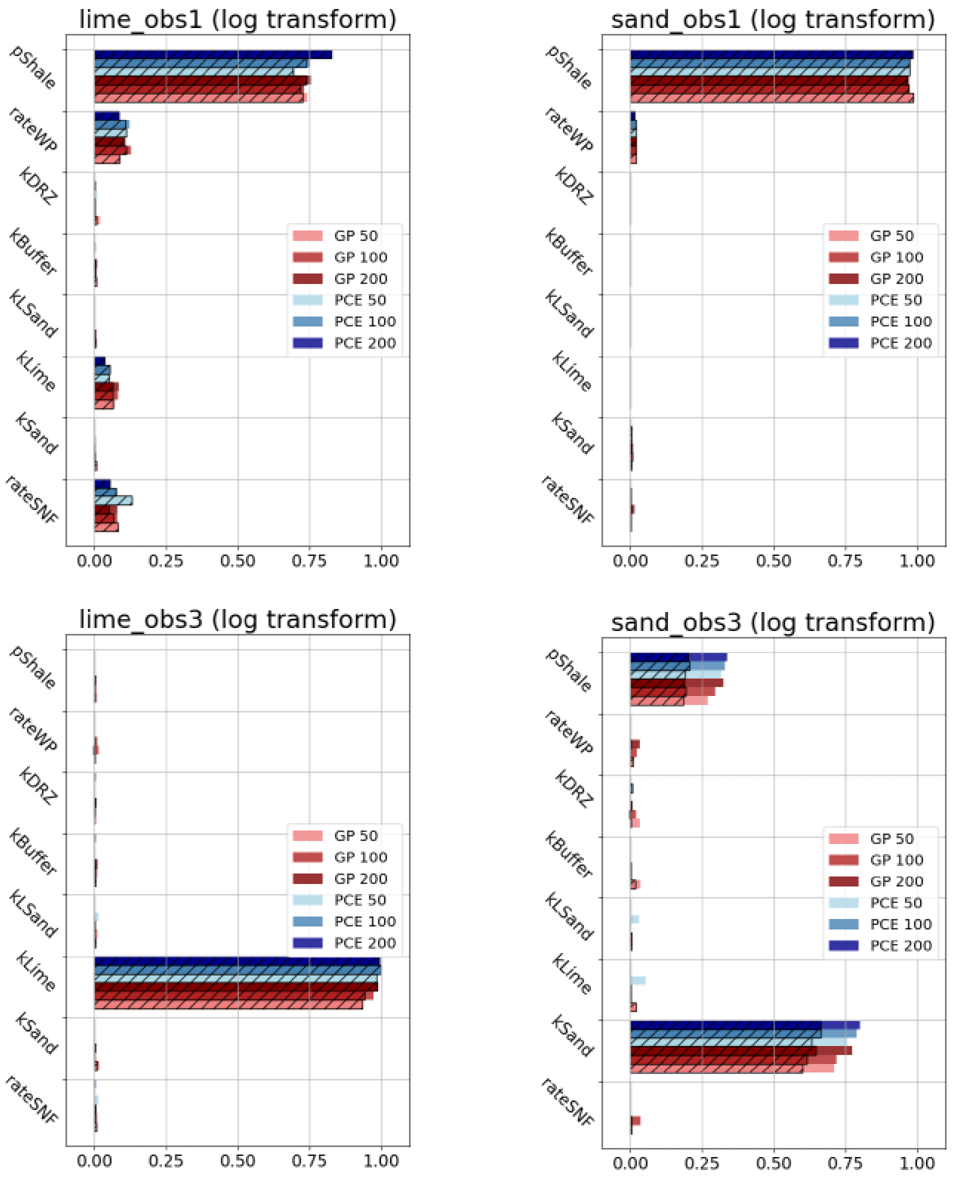
# Shale (argillite) reference case results

- **Regardless of method and sample size:**
  - Max [I-129] is sensitive to the porosity of the shale host rock (pShale).
  - Further from the repository, max [I-129] is sensitive to the permeability of the aquifer (kLime for lower and kSand for upper).
  - $S_T$ ~ 0 for kDRZ, kBuffer indicates values of these variables could be fixed without changing variance of the output.




I-129 concentration at 1,000,000 y plotted in a vertical slice at the Y-midpoint of the repository.

**Lower Aquifer** **Upper Aquifer**



# Results to date

- Statistical analyses over 100's of simulations have been conducted using DAKOTA and PFLOTRAN for three generic host rock types
- Model behavior appears realistic and methods are robust
- Across all three reference cases **aquifer properties** have significant impact on peak I-129 results
- Other quantities of interest for at least one of the cases is damage zone permeability (salt), fuel dissolution rate (crystalline), and porosity of the host formation (shale)

# Next steps

- Next 1-2 Years
  - Simulation and analysis of salt and crystalline reference cases developed in DECOVALEX Task F (next presentation)
  - Drive development of process models
    - Bentonite evolution
    - Waste package degradation
    - Salt consolidation and creep
- Longer term
  - Gas generation
  - Disruptive events

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