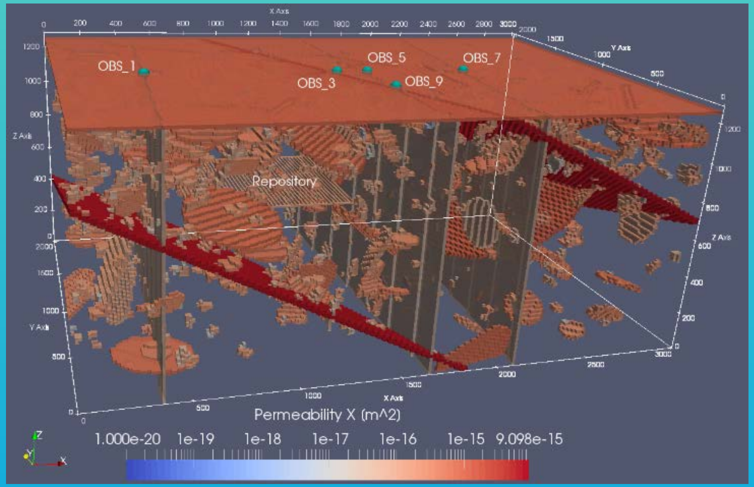

Reference Case Simulations

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

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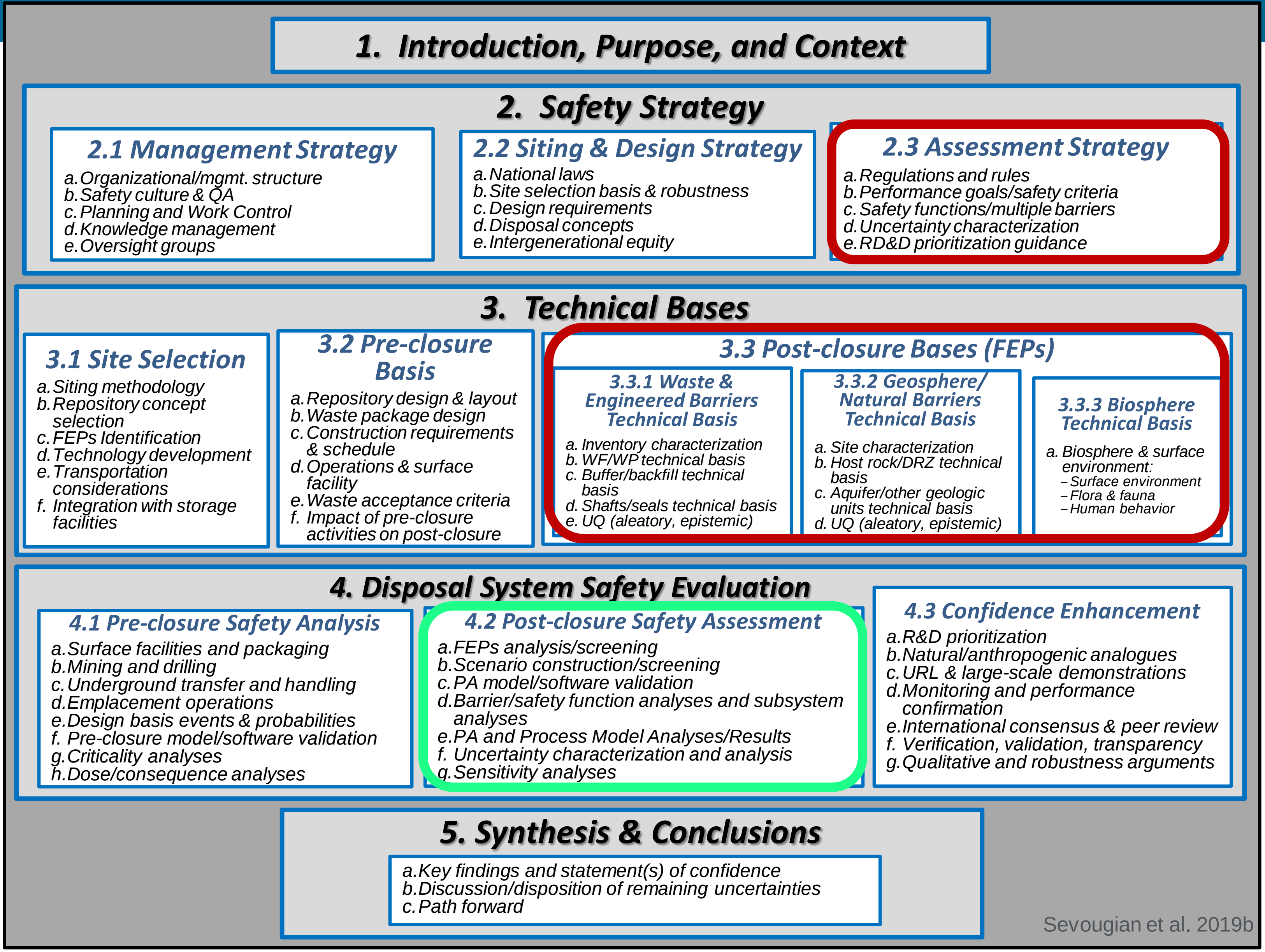
SAND2021-13707 PE

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

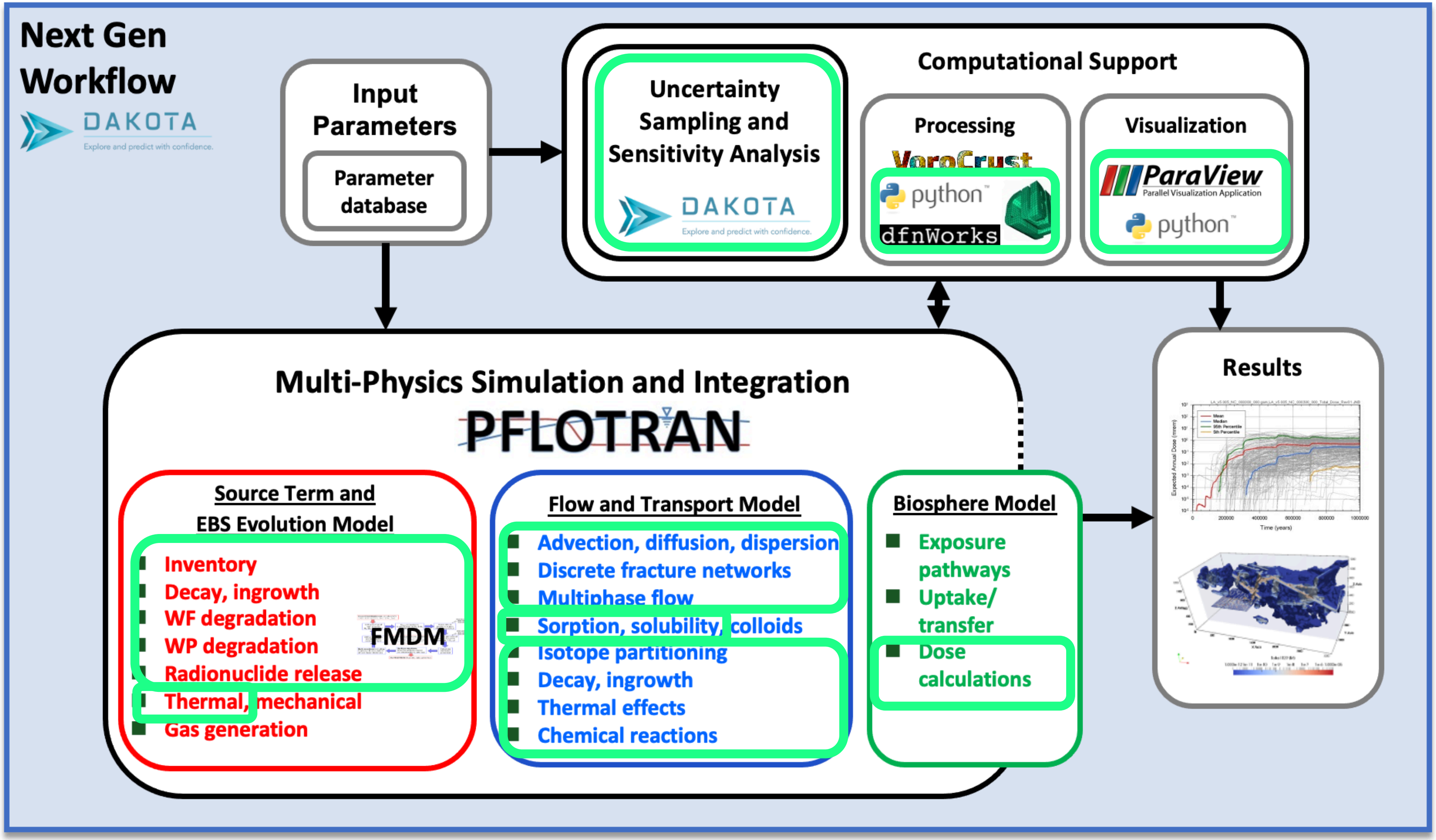
Sevougian et al. 2019b

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. 2019b

GDSA Framework



Next Gen Workflow

DAKOTA
Explore and predict with confidence.

Input Parameters

Parameter database

Computational Support

Uncertainty Sampling and Sensitivity Analysis

DAKOTA
Explore and predict with confidence.

Processing

VoroCrust
python
dfnWorks

Visualization

ParaView
Parallel Visualization Application
python

Multi-Physics Simulation and Integration

PFLOTRAN

Source Term and EBS Evolution Model

- Inventory
- Decay, ingrowth
- WF degradation
- WP degradation
- Radionuclide release
- Thermal, mechanical
- Gas generation

FMDM

Flow and Transport Model

- Advection, diffusion, dispersion
- Discrete fracture networks
- Multiphase flow
- Sorption, solubility, colloids
- Isotope partitioning
- Decay, ingrowth
- Thermal effects
- Chemical reactions

Biosphere Model

- Exposure pathways
- Uptake/ transfer
- Dose calculations

Results

Reference case simulations overview

- Overarching goal: Develop and demonstrate numerical modelling 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 I-129 in aquifer

Processes in all performance assessment models

- Coupled heat and fluid flow
- Radionuclide transport via advection and diffusion
- Radionuclide sorption using linear distribution coefficients (K_d)
- Radionuclide precipitation/dissolution
- Radioactive decay and ingrowth in all phases
- Waste package degradation
- Waste form dissolution

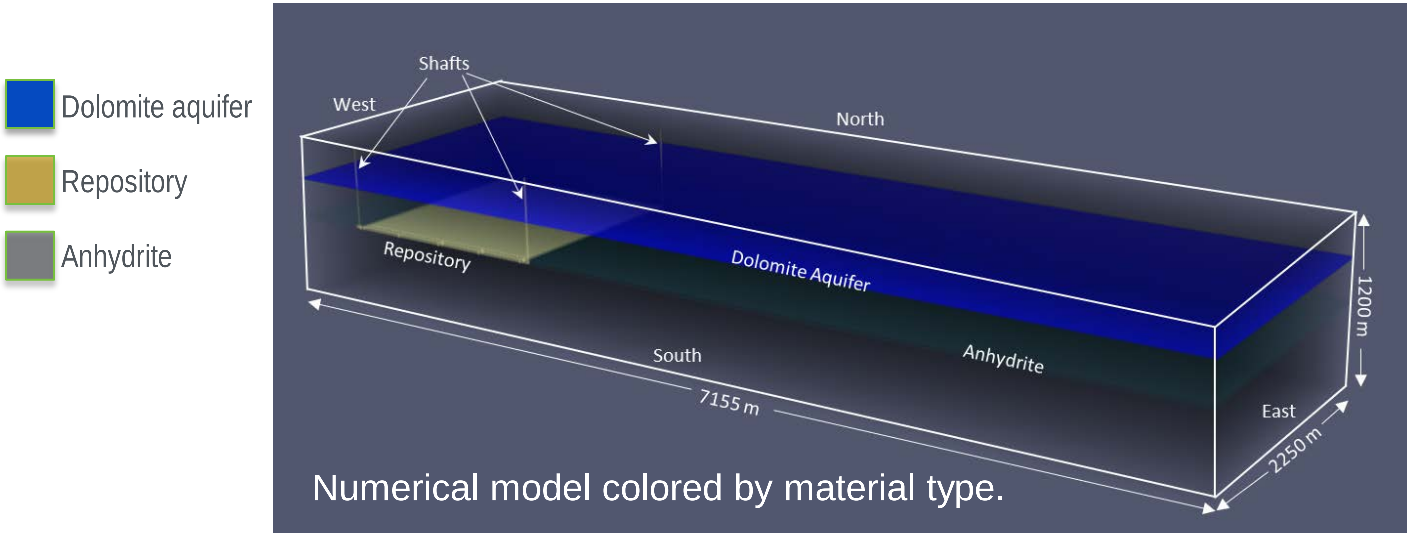
Reference case simulation overview – generic concepts

		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	**≤ 1 kW**	**1 kW**	**3 kW**	**4 kW**	**4 & 6 kW**
	Max Temperature	**100° C**	**105° C**	**150° C**	**250° C**	**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	**≤ 1 kW**	**1 kW**	**3 kW**		
	Max Temperature	**85° C**	**100° C**	**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	**≤ 1 kW**		**6 kW**	**10 kW**	**7 & 9 kW**
	Max Temperature	**90° C**		**150° C**	**200° C**	**120° & 150°**

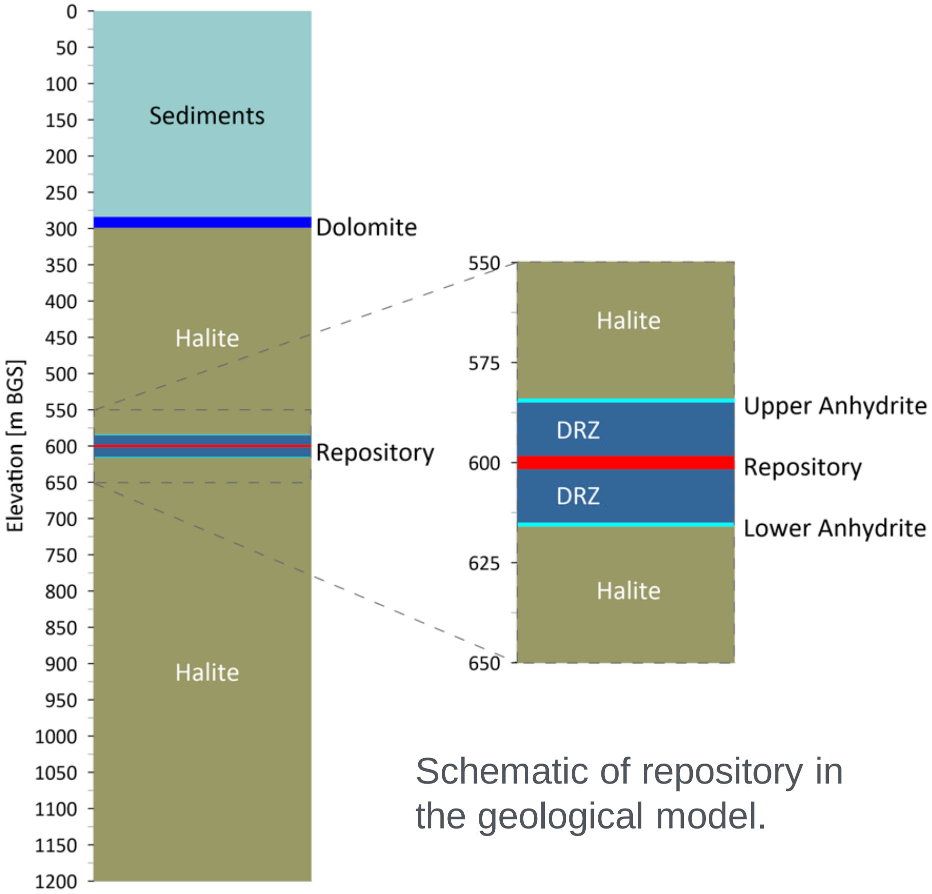
κ = thermal conductivity (of the liquid-saturated host rock)
SNF = spent nuclear fuel
HLW = high level waste
CSNF = commercial spent nuclear fuel
PWR = pressurized water reactor (assembly); represents waste package capacity

Salt reference case (LaForce et al, 2020)

- 3100 24- pressurized water reactor assembly (PWR) and 2000 37-PWR waste packages in 102 drifts
- Numerical model is a half-symmetry domain with 9.2 million grid cells
- Geological features:
  - 0.0013 [m/m] head gradient from west to east
  - Anhydrite layers above and below the repository,
  - adjacent to the disturbed rock zone
  - Dolomite aquifer overlies the repository



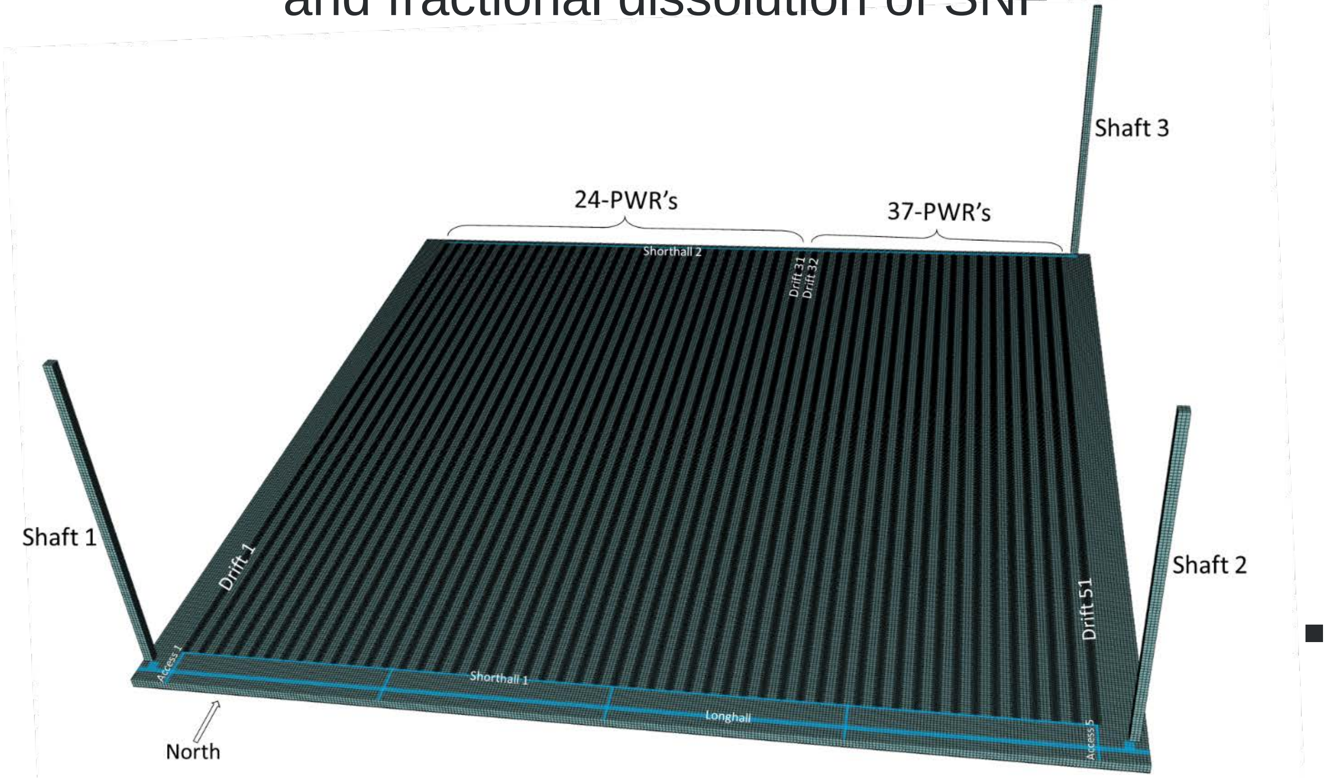
Numerical model colored by material type.



Schematic of repository in the geological model.

Salt reference case (LaForce et al, 2020)

- Repository features
  - Run-of-mine salt backfill
  - Instant-release fraction for I-129 of 0.10 and fractional dissolution of SNF

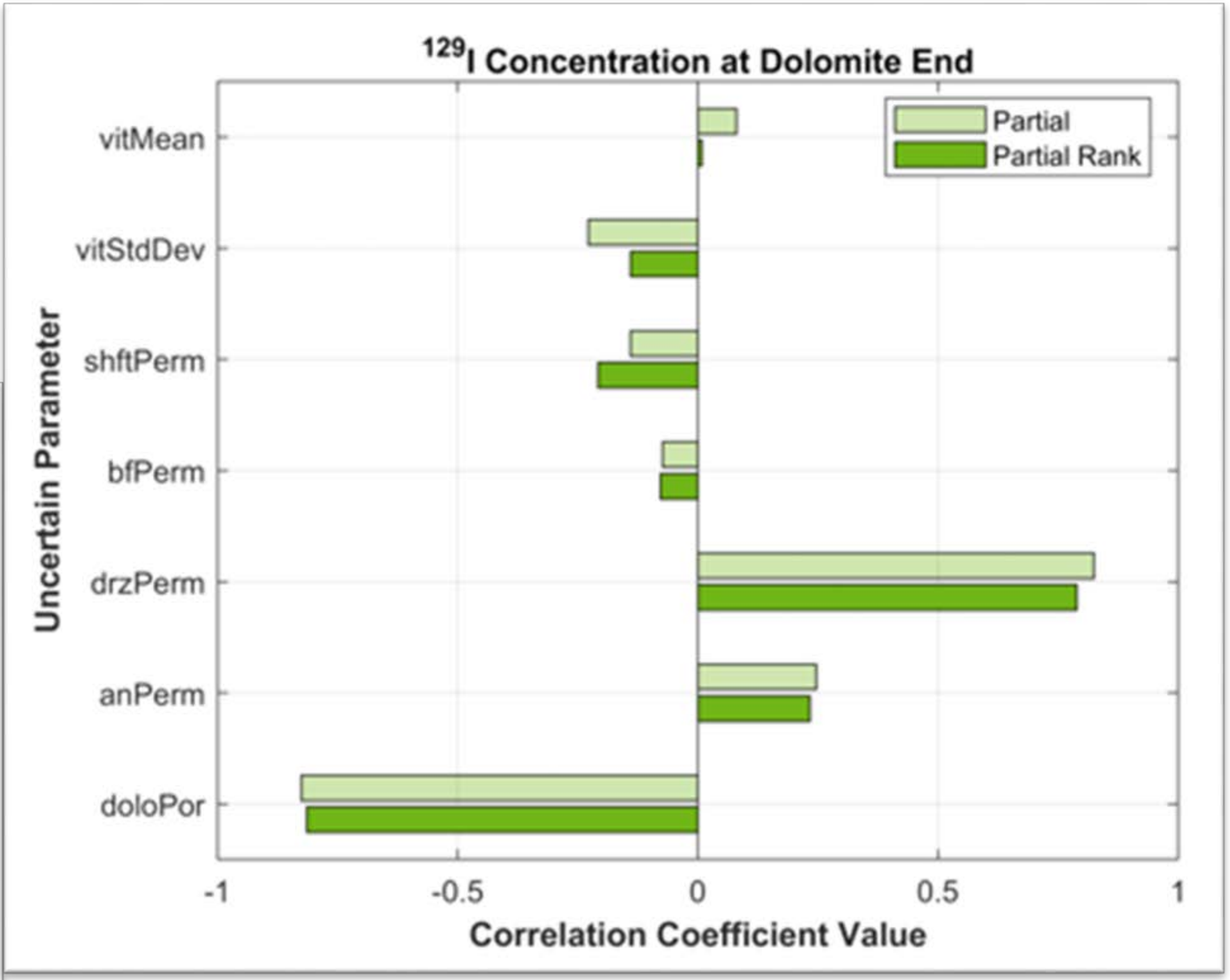


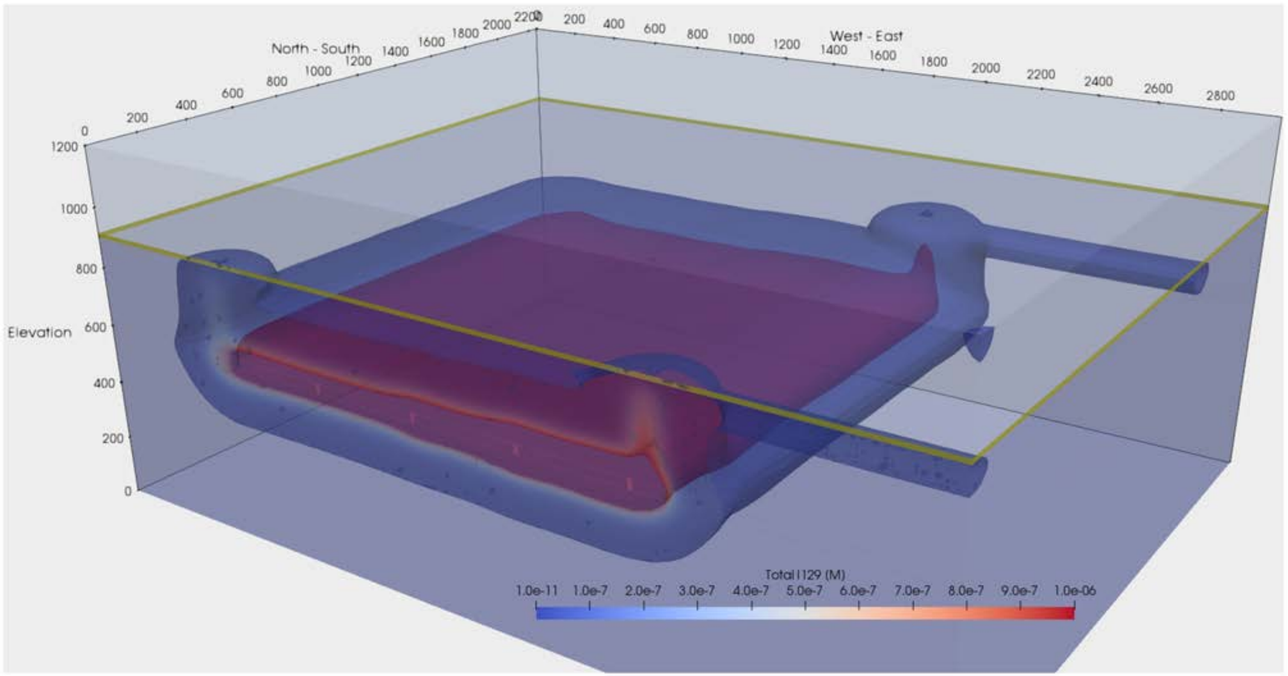
Half of the repository colored by material type.

- 200 simulations with uncertain parameters sampled using Dakota's Latin hypercube sampling (LHS)
- 7 sampled parameters are:
  - Natural barrier properties
    - Porosity of the dolomite
    - Permeability of the anhydrite
    - Permeability of the disturbed rock zone (DRZ)
  - Engineered barrier properties
    - Backfill permeability
    - Shaft permeability
    - Mean and standard deviation of the waste package degradation rate coefficient
- Performance metric is maximum I-129 in dolomite aquifer 5km downstream of repository

Salt reference case results (LaForce et al, 2020)

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

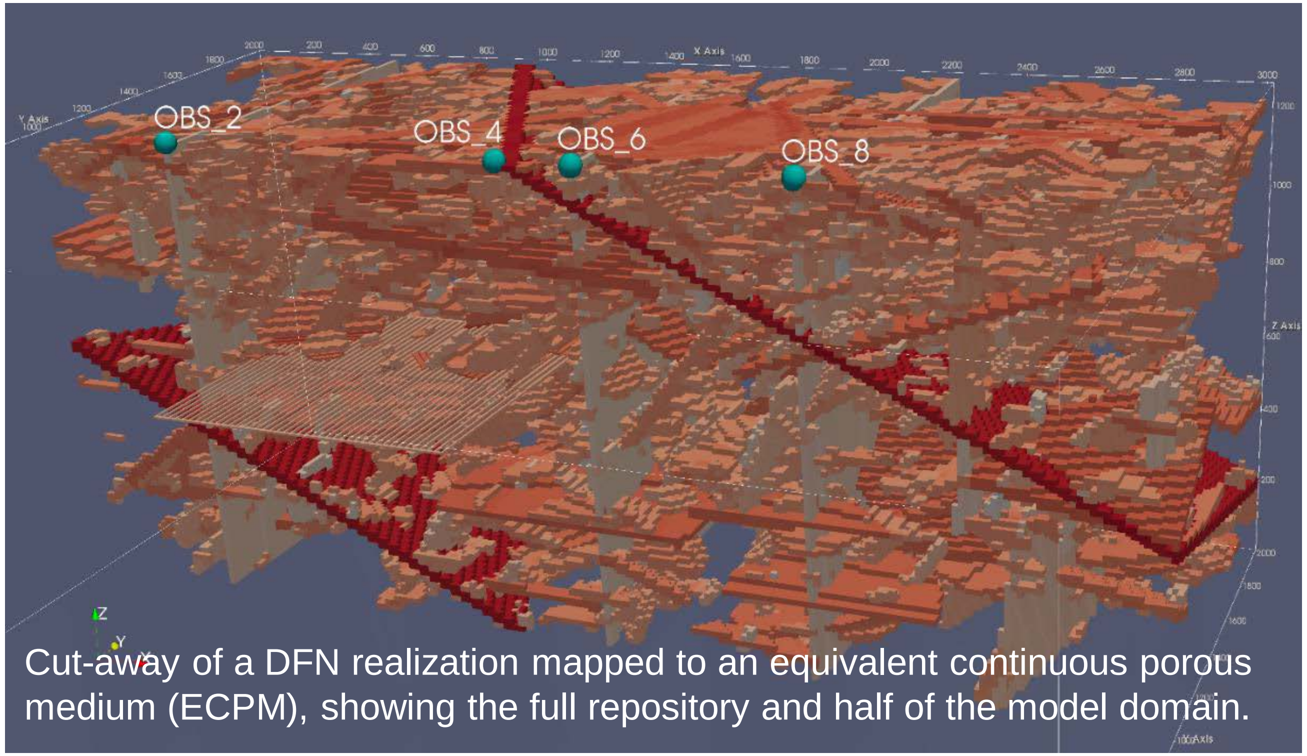




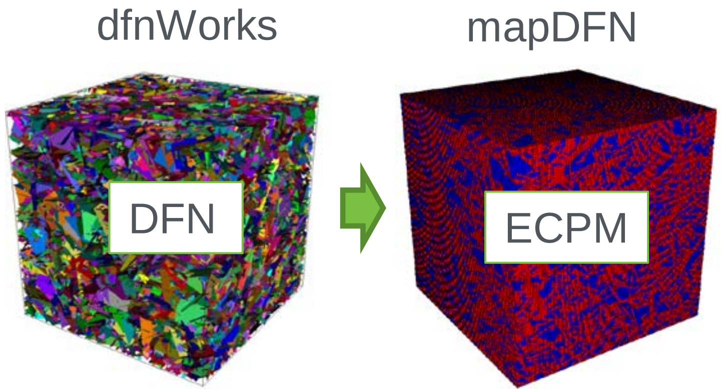
^{129}I concentration after 1,000,000 years (10^{-11} to 10^{-6} M shown)

Crystalline reference case (Swiler et al. 2021)

- 1680 12-PWR waste packages in 42 disposal drifts
- Geological features:
  - 0.0013 (m/m) head gradient from west to east
  - Deterministic and stochastic fracture network
  - Sedimentary aquifer overlies the repository
- Numerical model features
  - 4.8 million grid cells
  - I-129 as radionuclide of interest
  - Discrete fracture networks (DFNs)

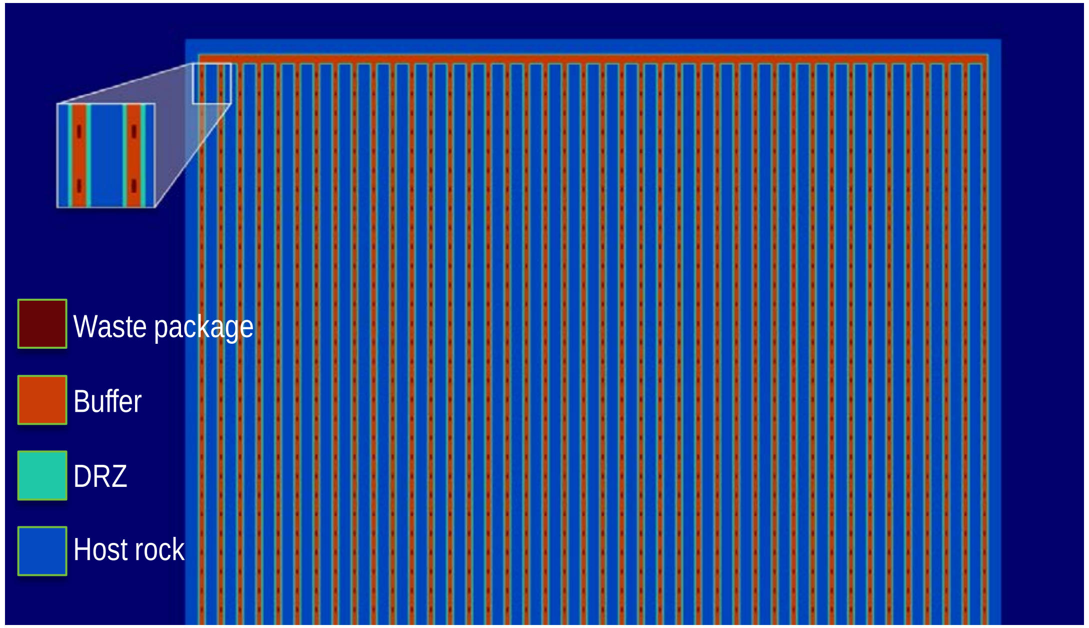


Cut-away of a DFN realization mapped to an equivalent continuous porous medium (ECPM), showing the full repository and half of the model domain.



Crystalline reference case (Swiler et al, 2021)

- Repository features
  - Bentonite backfill
  - Instant-release fraction for I-129 and fractional dissolution of SNF

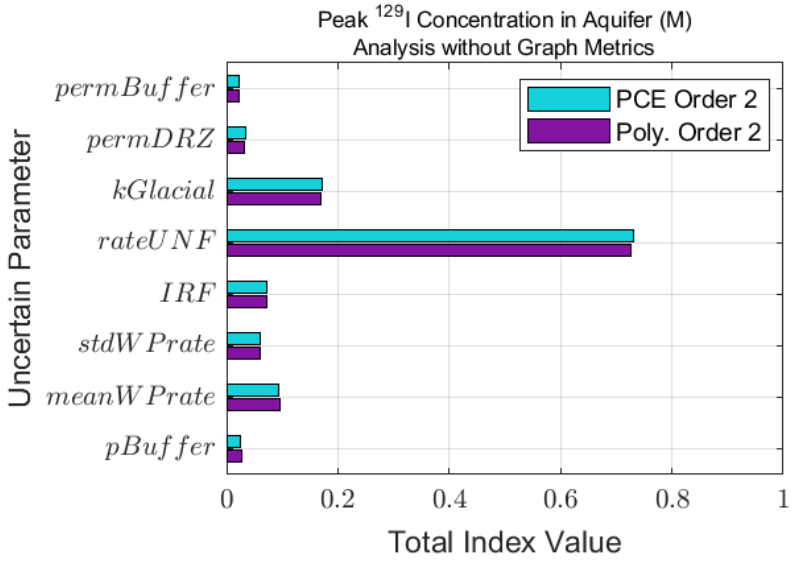


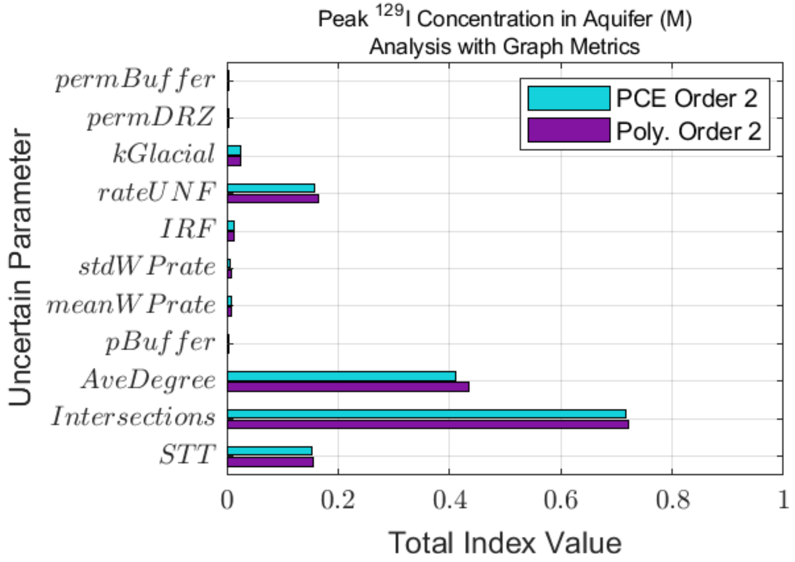
Map view of part of the repository colored by material type.

- 1000 simulations with uncertain parameters sampled using LHS
- 25 realizations of discrete fracture network
- 8 sampled parameters are:
  - Natural barrier properties
    - Permeability of the disturbed rock zone
    - Permeability of overlying aquifer
  - Engineered barrier properties
    - Porosity and permeability of bentonite buffer
    - Mean and standard deviation of the waste package degradation rate coefficient
    - Fuel dissolution rate
    - Instant release fraction upon waste package breach
- Performance metric is element-wise maximum I-129 in aquifer

Crystalline reference case results

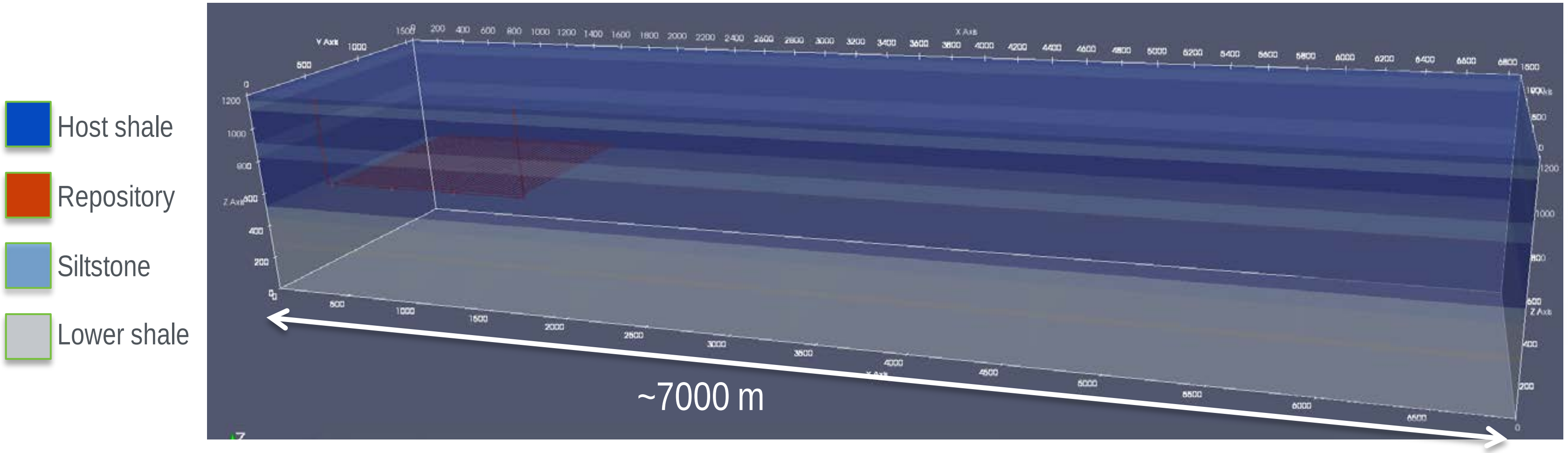
- Total sensitivity indices
- When stochastic variation in the fracture network is not considered in the sensitivity analysis:
  - Peak I-129 concentration appears most sensitive to the rate of spent nuclear fuel dissolution
- When stochastic variation in the fracture network is considered in sensitivity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



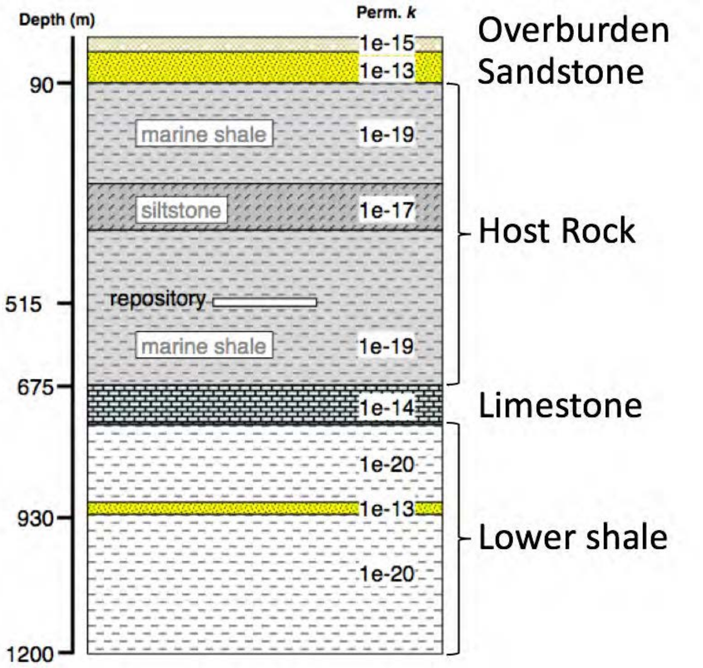


Shale (argillite) reference case (Mariner et al. 2017; Swiler et al. 2019)

- 4200 12-PWR waste packages in 84 drifts
- Numerical model is a half-symmetry domain with 6.9 million grid cells
- Geological features:
  - 0.0013 (m/m) head gradient from west to east
  - Sandstone aquifer above the repository
  - Limestone aquifer below the repository



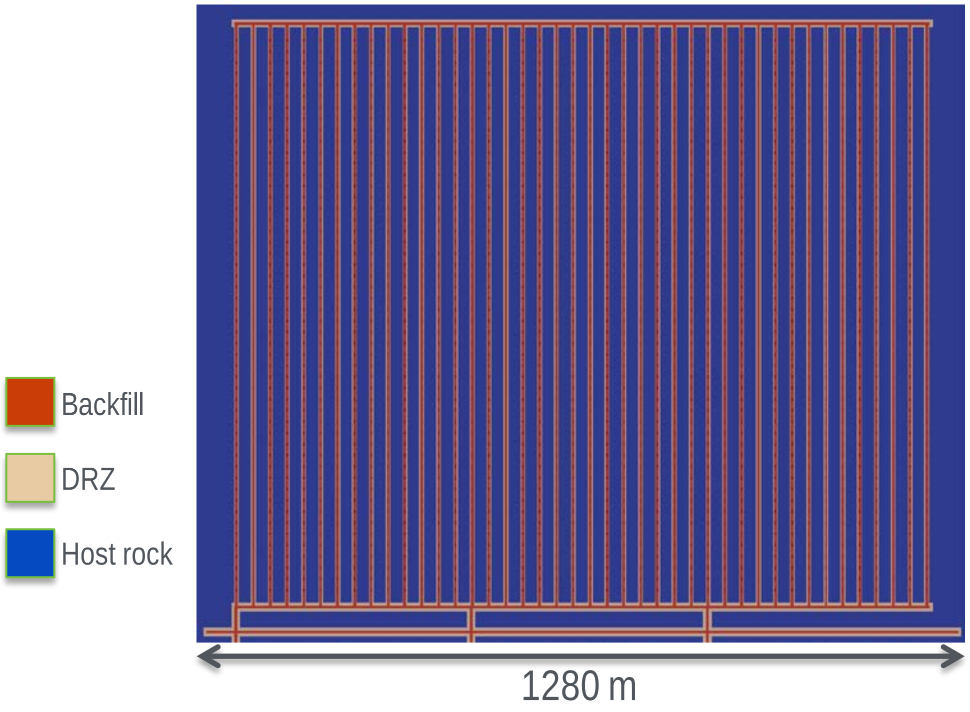
Numerical model colored by material type.



Schematic of repository in geological model.

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

- Repository features
  - Bentonite backfill
  - Instant-release fraction for I-129 of 0.10 and fractional dissolution of SNF



Map view of half of the repository colored by material type.

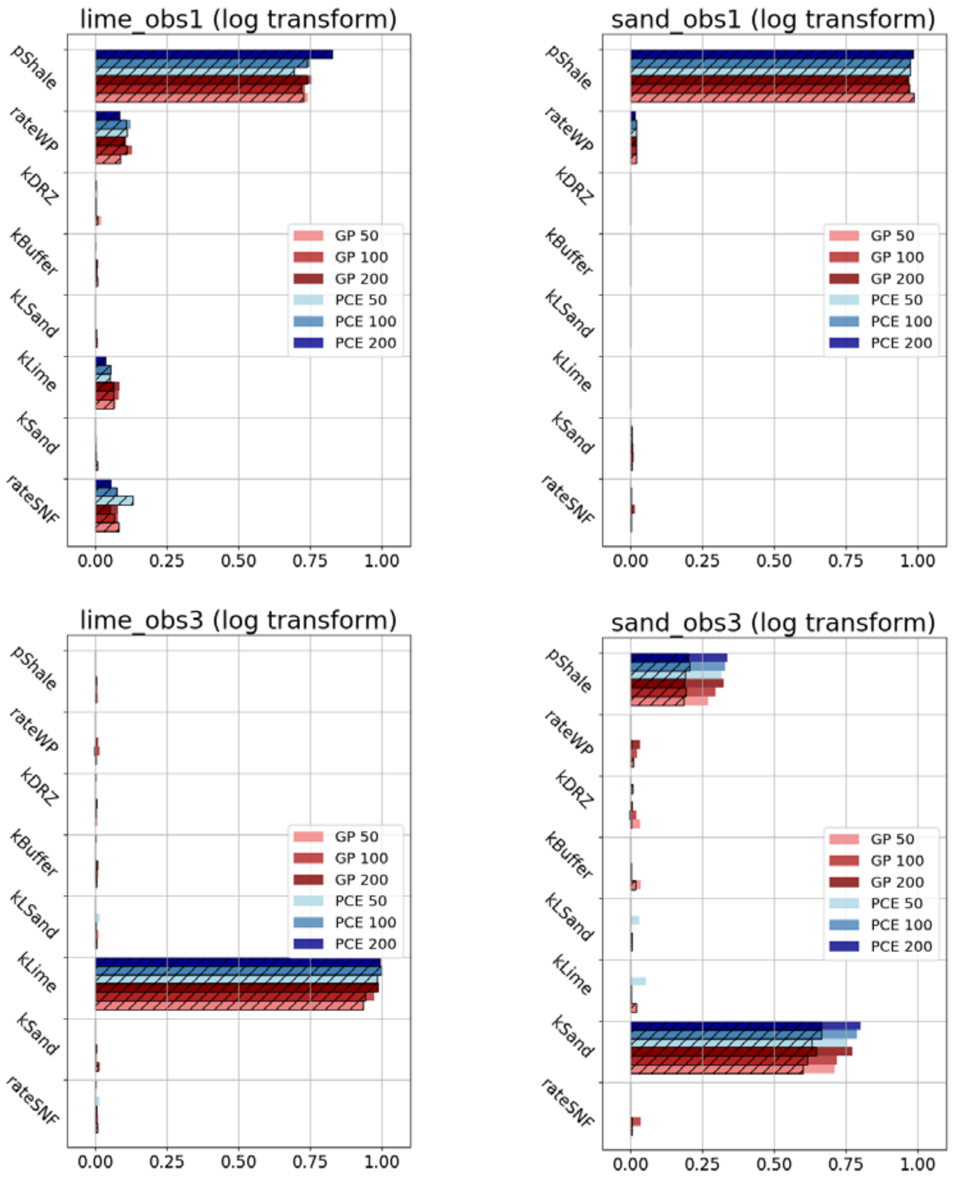
- Incremental LHS sampling of uncertain parameters with an initial sample size of 50 and a final sample size of 200
- 10 sampled parameters are:
  - Natural barrier properties
    - Permeability of
      - Underlying limestone aquifer
      - Overlying sandstone aquifer
      - Lower sandstone aquifer
      - Disturbed rock zone
    - Porosity of host shale
    - Np-237 K_d in buffer and shale (not used)
  - Engineered barrier properties
    - Permeability of bentonite buffer
    - Mean waste package degradation rate coefficient
    - Fuel dissolution rate
- Performance metric is maximum I-129 in aquifers 5km downstream of repository

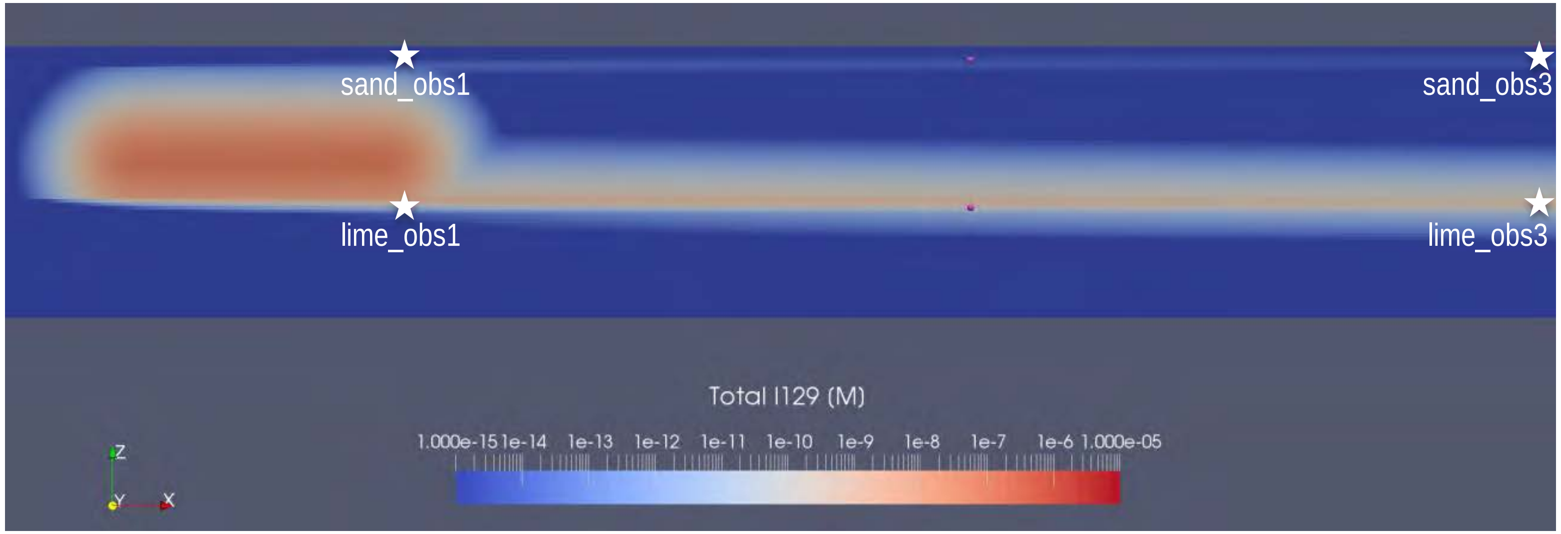
Shale (argillite) reference case results

- **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.

Lower Aquifer

Upper Aquifer





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

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 disturbed rock zone permeability (salt), fuel dissolution rate (crystalline), and porosity of the host formation (shale)

Next steps

- Next 1-2 Years
  - Numerical modelling 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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