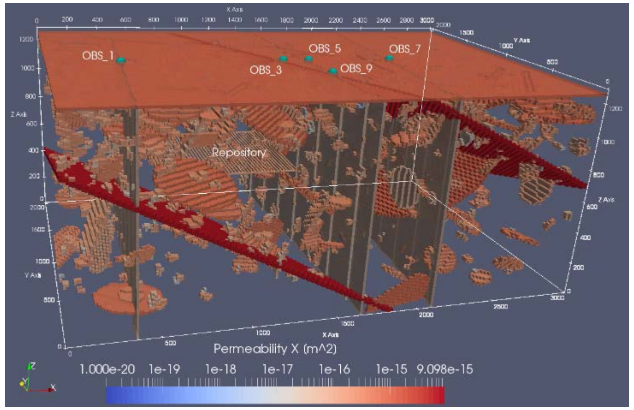

GDSA R&D Activities Related to Crystalline Host Rock

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Sandia National Laboratories

U.S. NWTRB Meeting

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Spent Fuel and Waste Science and Technology (SFWST)

Outline

- **GDSA activities for crystalline rock**
- **Crystalline repository reference cases**
- **Specific modeling in GDSA crystalline reference case**
  - Excavation effects
  - Buffer erosion
- **DECOVALEX crystalline reference case**
- **Performance factor analysis**

GDSA Modeling Objectives

- **Develop modeling capabilities that support simulation of coupled processes controlling disposal system performance**
- **The modeling capability will:**
  - Integrate conceptual models of subsystem processes and couplings
  - Incorporate reasonable ranges of site characterization data
  - Propagate uncertainty

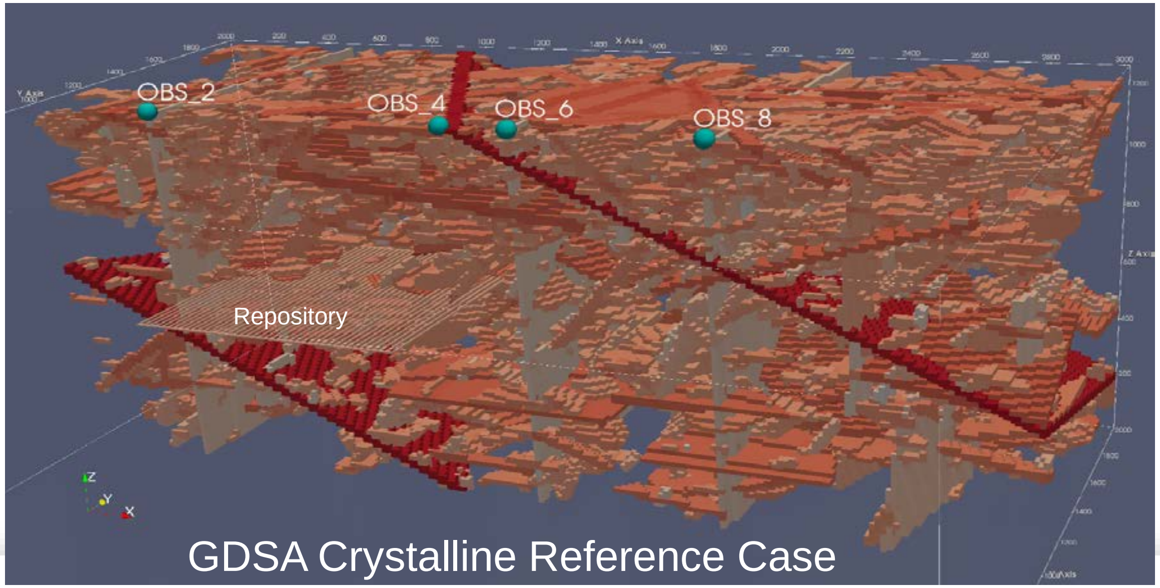
GDSA R&D Activities – Crystalline

- **GDSA Framework capability development (crystalline)**
  - Discrete fracture network (DFN) modeling (Stein et al. 2017)
  - Dual Continuum Disconnected Matrix (DCDM) model (Nole et al. 2022)
  - Buffer erosion / canister corrosion model (Nole et al. 2022)
  - Performance factor analysis of engineered barriers (Mariner et al. 2024)
  - Tracking tool to assess Features, Events, and Processes (FEPs) coverage for a reference case and identify gaps (Mariner et al. 2023)
  - Continued progress in automation, reproducibility, and transparency of probabilistic reference case simulations and sensitivity analyses (Swiler et al. 2023)
- **Crystalline reference case development and simulation**
  - International comparison of performance assessment model capabilities (DECOVALEX-2023 Task F1 – crystalline host rock) (LaForce et al. 2023)
  - GDSA crystalline reference case development and sensitivity analyses (Stein et al. 2017; Mariner, Stein et al. 2016; Swiler et al. 2021)

Crystalline Repository Reference Cases

- **GDSA Crystalline Reference Case**
  - 3 km x 2 km x 1.3 km
  - Overlying glacial aquifer
  - Groundwater flow: west face to east face
  - Repository at 600 m
  - In-drift emplacement, 12-PWR waste packages
  - Non-isothermal
  - Fracture network upscaled to equivalent continuous porous medium (ECPM)

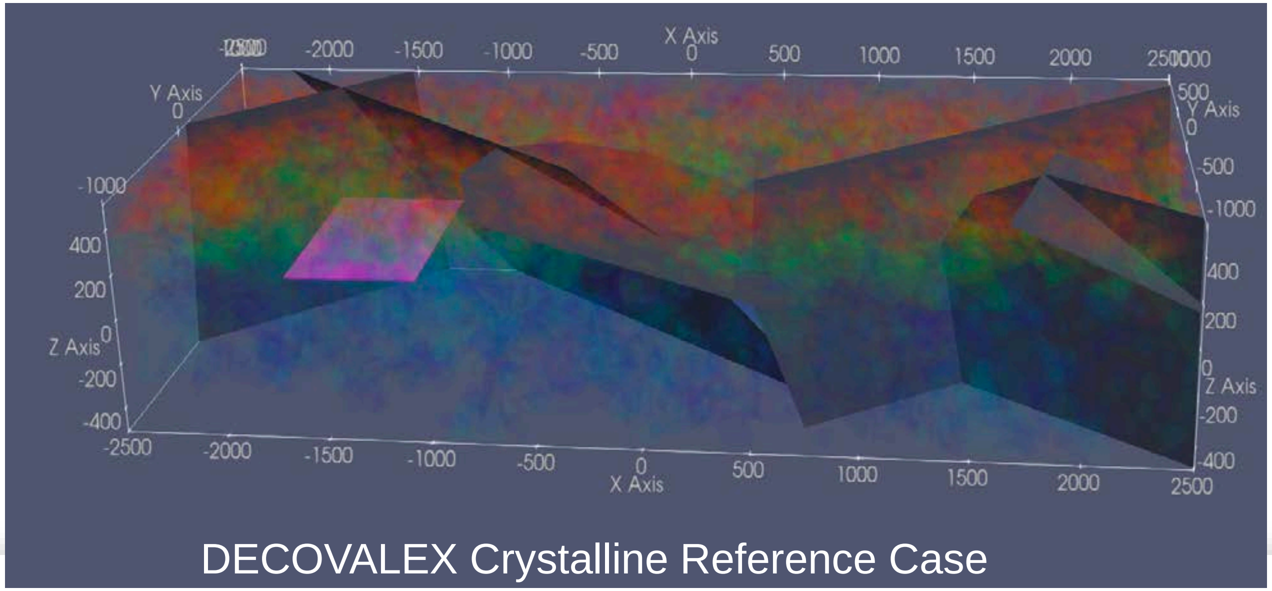
Stein et al. (2017)



GDSA Crystalline Reference Case

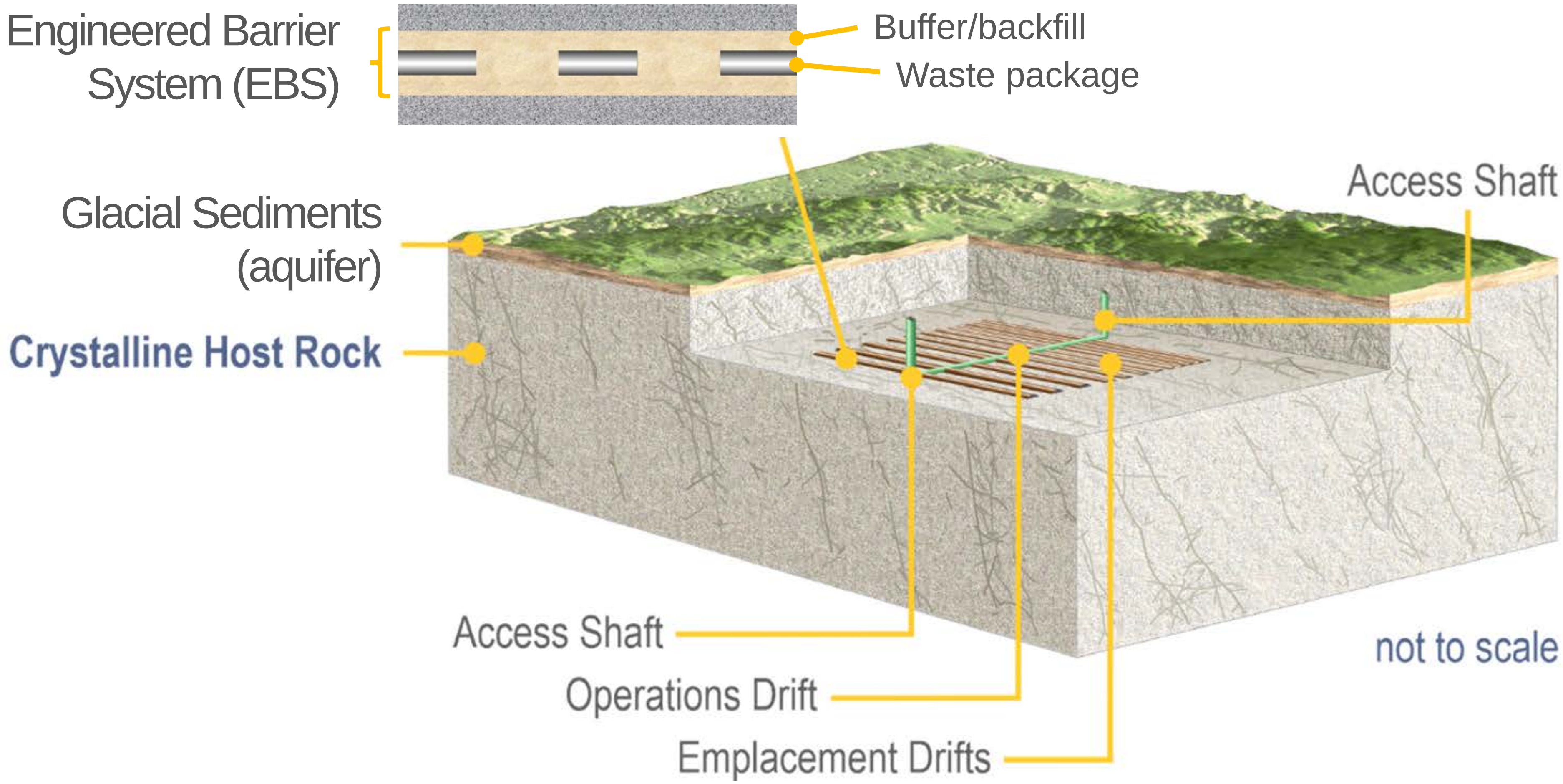
- **DECOVALEX Crystalline Reference Case**
  - 5 km x 2 km x 1 km
  - Higher ground in west, lower ground in east
  - Groundwater flow: downward in west, upward in east
  - Repository at 450 m
  - Deposition holes (KBS-3V), 4-PWR waste packages
  - Isothermal
  - Depth-dependent fracture network upscaled to equivalent continuous porous medium (ECPM)

Leone et al. (2024)



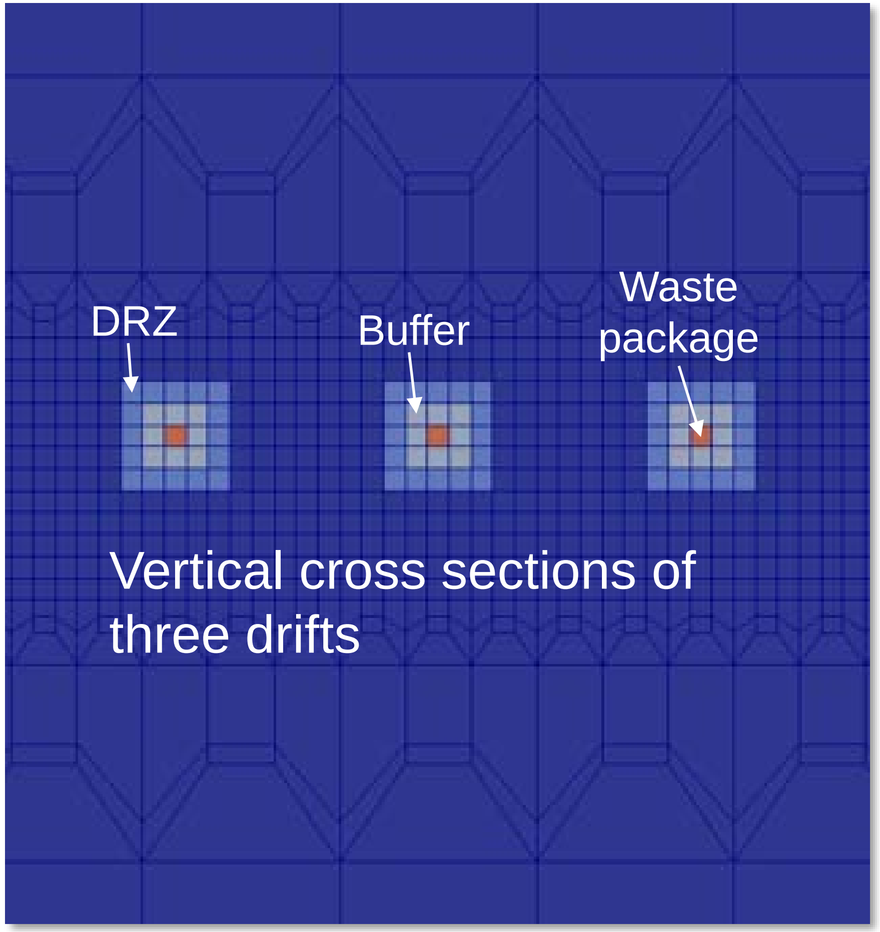
DECOVALEX Crystalline Reference Case

GDSA Crystalline Repository



GDSA Crystalline Drifts & DRZ

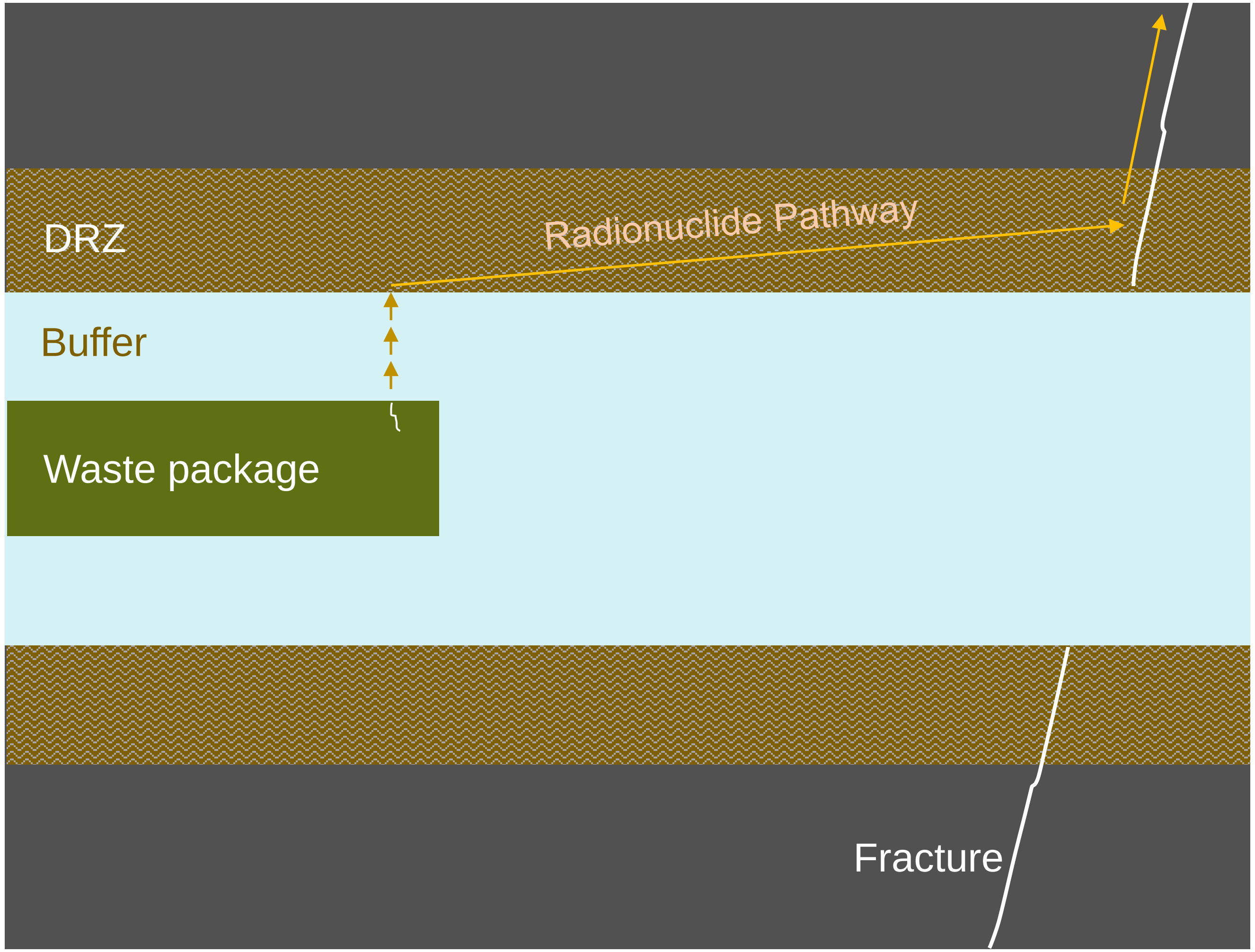
- **42 disposal drifts**
  - 20 m center-to-center spacing
  - 12-PWR waste packages (WPs)
  - Bentonite buffer backfill
- **Excavation effects**
  - Simulated using DRZ
    - DRZ = damaged rock zone
  - DRZ thickness: 1.67 m at all walls
    - Supported by observations at the Korean Underground Research Tunnel (Cho et al. 2013)



Stein et al. (2017)

DRZ in GDSA Crystalline Reference Case

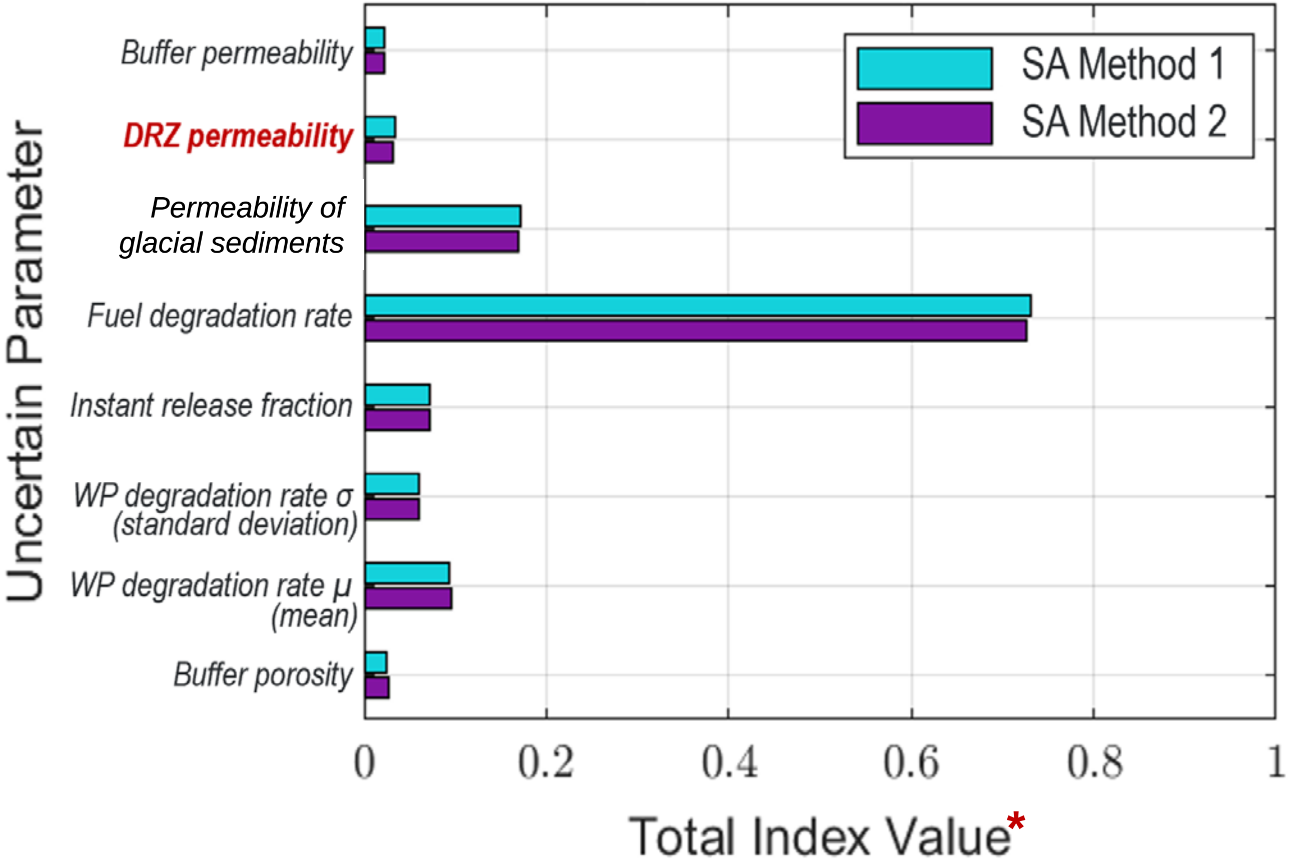
- **Emulate increased fracturing**
- **DRZ cell properties**
  - Permeability: 10^{-19} to 10^{-16} m^2
    - Cho et al. (2013); Martino and Chandler (2004)
    - Host rock: 10^{-20} m^2
  - Porosity: 1%
    - Host rock : 0.5%
  - Effective diffusion coefficient: 10^{-11} m^2
    - Host rock : 10^{-12} m^2
- **DRZ effects**
  - Increases fracture connections
  - Enhances groundwater flow around repository
  - Facilitates radionuclide migration to flowing fractures



Effects of DRZ in GDSA Reference Case

- **Effects of DRZ on performance**
  - E.g., on peak ^{129}I concentration in overlying glacial sediments
- **Sensitivity analysis (SA)**
  - Varied the DRZ permeability
    - 10^{-19} to 10^{-16} m^2 (log-uniform)
  - For this reference case, as modeled, DRZ permeability effects are small relative to other parameters

Peak ^{129}I Concentration in Glacial Sediments

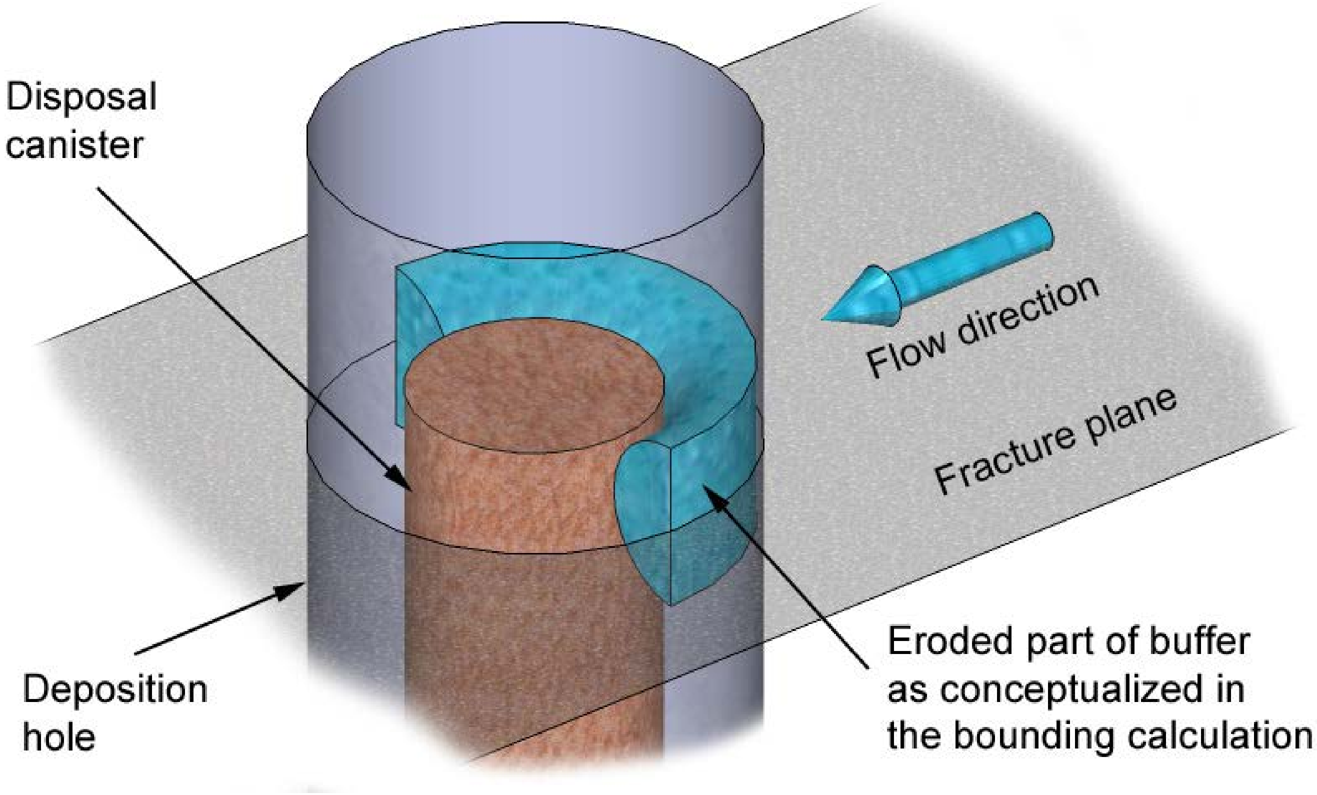


Swiler et al. (2021)

*Total Index Value indicates peak ^{129}I relative variance owing to the uncertain parameter and its interactions with other uncertain parameters

Buffer Erosion Model in GDSA

- **Conceptual model**
    - Neretnieks et al. (2017)
  - Flowing fracture intersects drift or deposition hole (see figure)
  - If ionic strength low (<0.004 M)
    - Buffer erosion
    - Otherwise, no buffer erosion
  - Buffer erosion rate is a function of
    - Fracture aperture and angle
    - Water velocity in fracture
    - Diffusion of colloidal particles
- **Capability**
  - Being implemented in PFLOTRAN
- **Inclusion in reference case**
  - Expected in future



Conceptual model of buffer erosion due to a flowing fracture (Posiva 2013)

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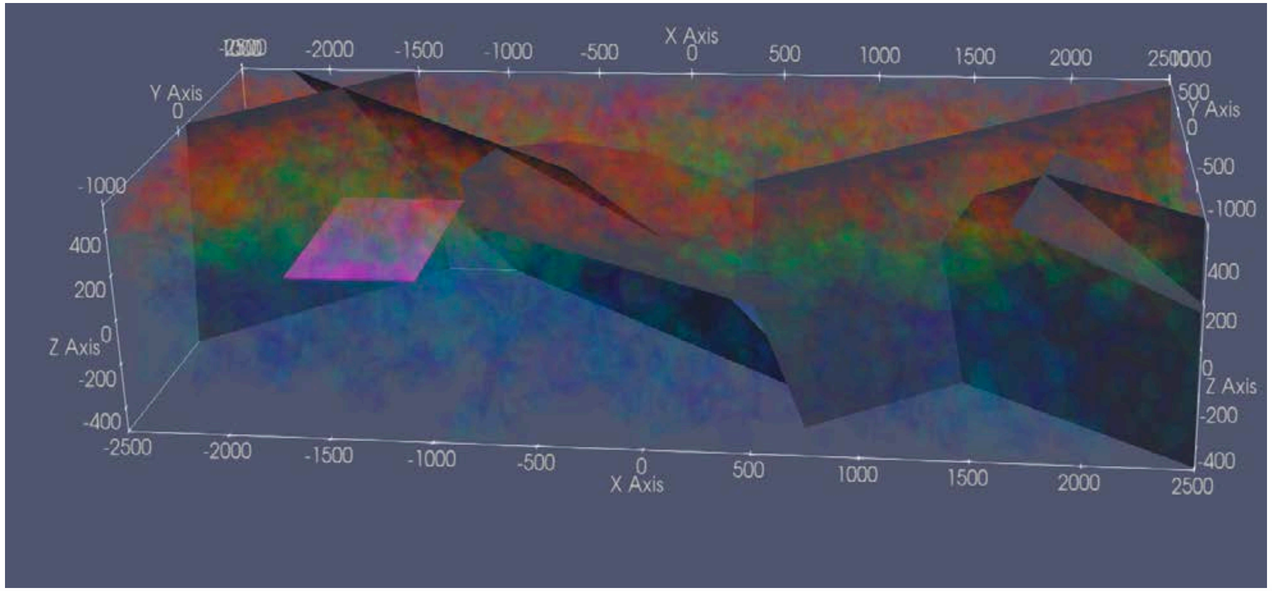
DECOVALEX Crystalline Reference Case

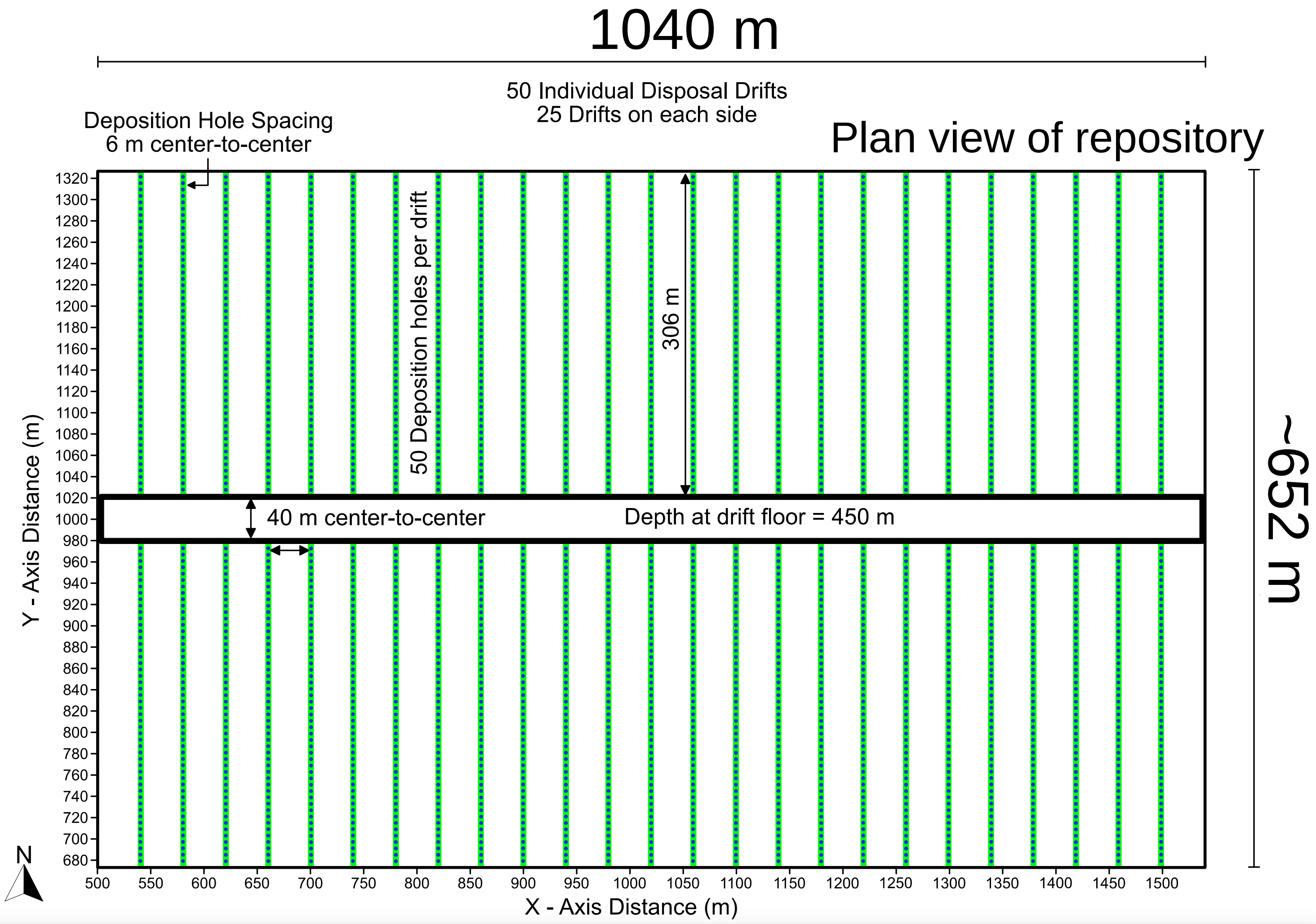
DECOVALEX Crystalline Reference Case

- **International research and model comparison collaboration**
- **Task F1: Generic crystalline repository**
- **Objectives: Build confidence in models, methods, and software used for Performance Assessment (PA)**
- **7 teams modeled full reference case**



DECOVALEX Crystalline Reference Case

- **50 Disposal Drifts**
  - 40 m center-to-center spacing
  - 4-PWR waste packages
  - Bentonite buffer backfill
- **Fracture network**
  - Loosely based on Olkiluoto
  - 10 fracture realizations
- **Steady state flow**
  - Top of domain simulates hillslope
- **Conservative tracers**



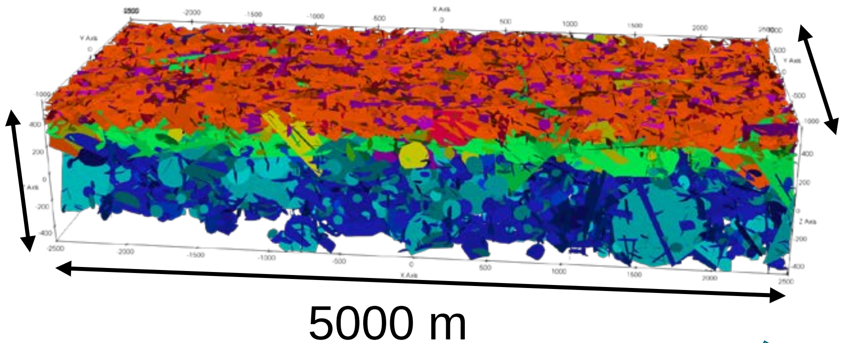
DFN Generation and Upscaling

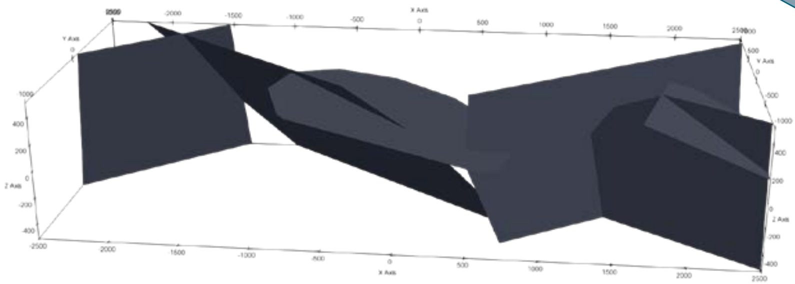
Fracture statistics (provided to teams):

- Pole orientation
  - Mean trend
  - Mean plunge
  - Concentration
- Power-law distribution
- Intensity of open flowing fractures
- Transmissivity

DFNWorks

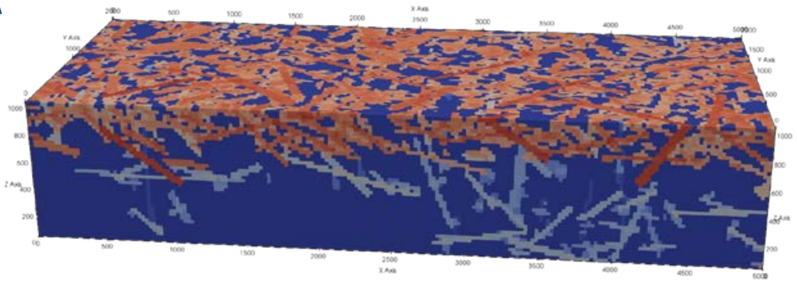
Stochastic Fractures





Deterministic Fractures

Equivalent Continuous Porous Medium (ECPM)



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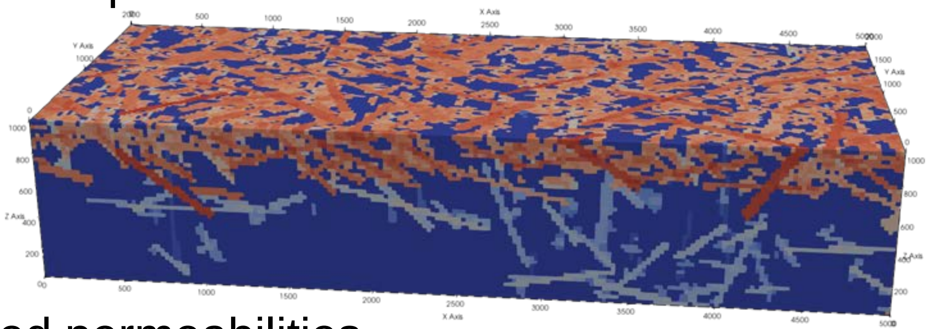
Upscaling Options

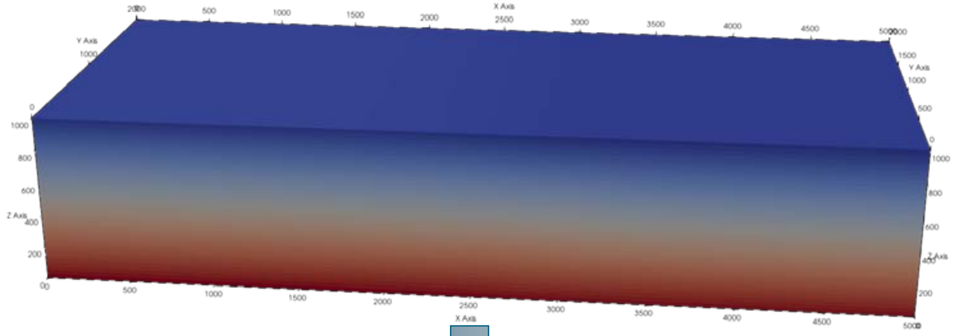
Principle component of permeability tensor passed to PFLOTRAN

ECPM

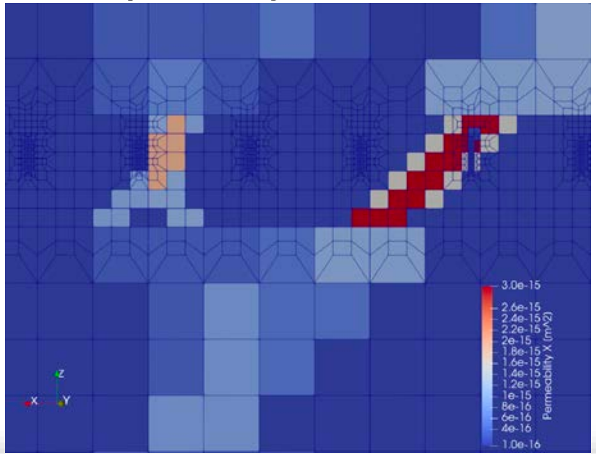


Permeability

Steady State Pressure Solution



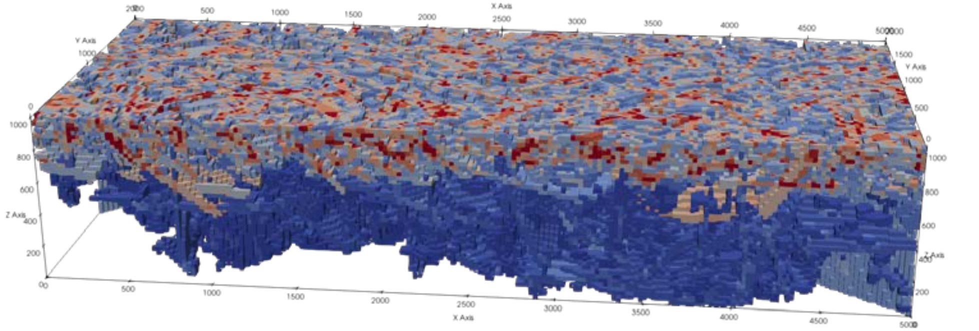
Slice of upscaled permeabilities in the repository



Options:

- Grid cell size/number
- Stairstep correction
- Dual continuum

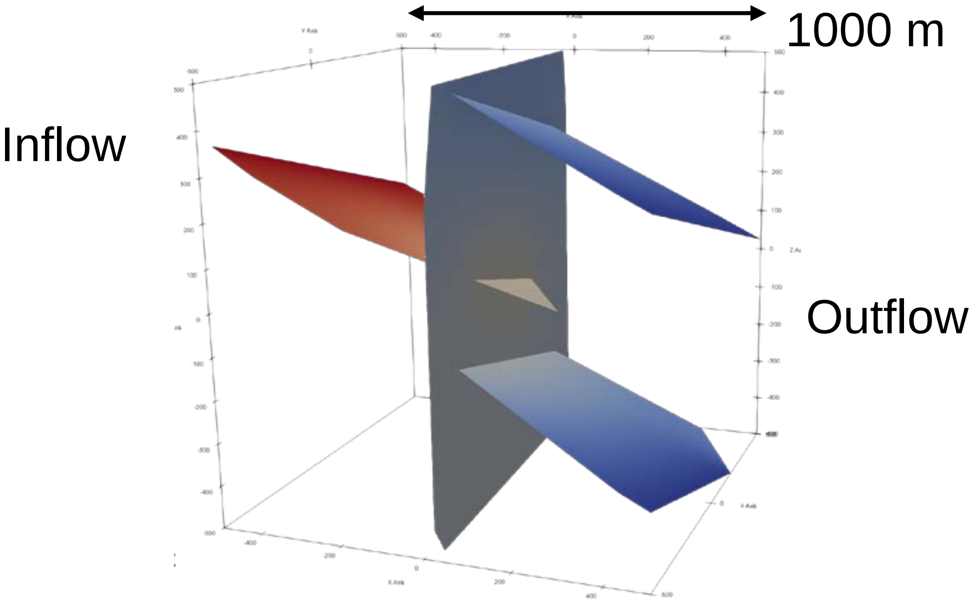
Dual Continuum in PFLOTRAN

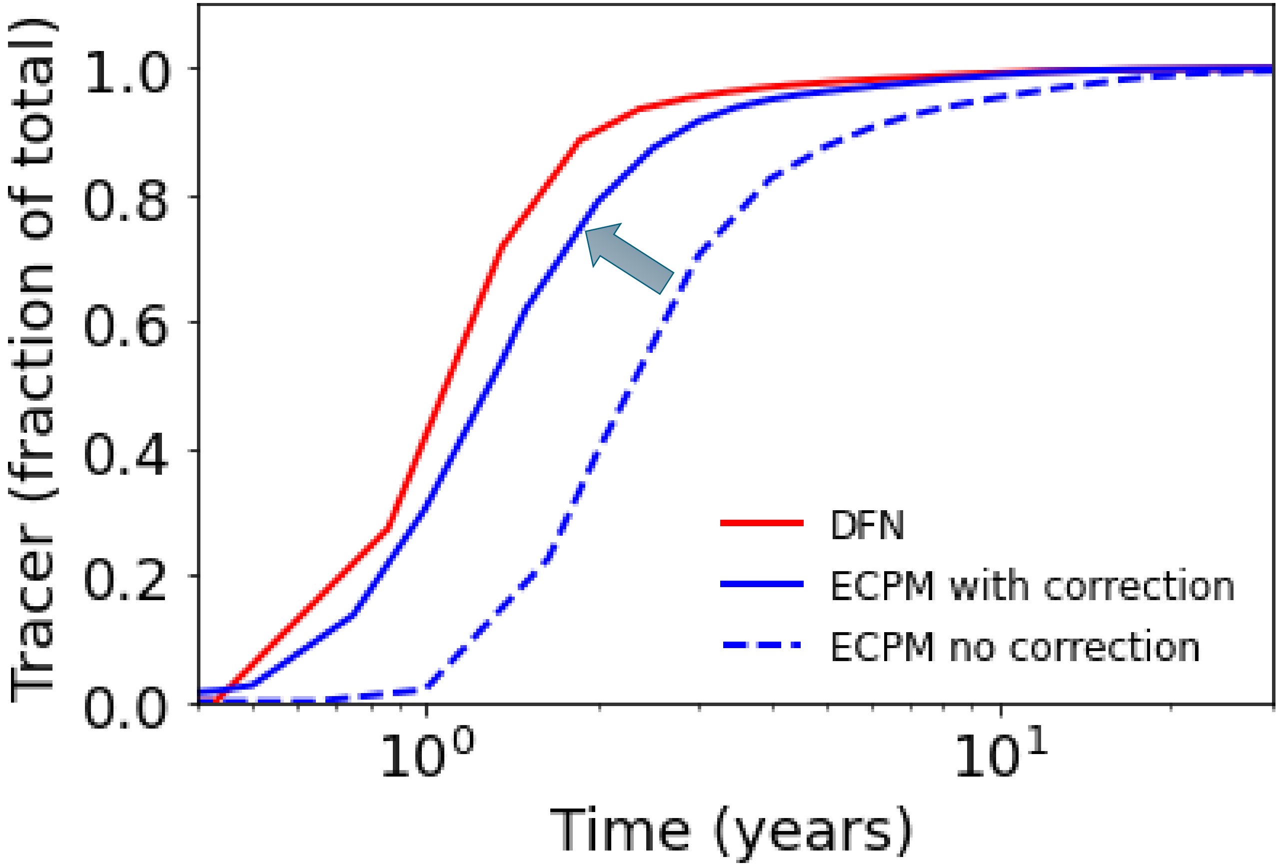


Fracture-matrix diffusion via Dual Continuum Discretized Matrix (DCDM) method

DECOVALEX Benchmark Case

- **Four deterministic fractures**
  - Stairstep correction improves comparison of DFN versus ECPM

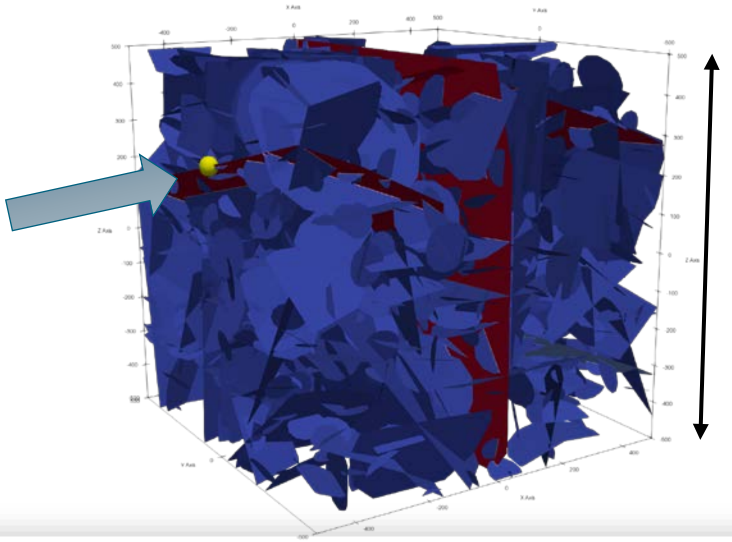




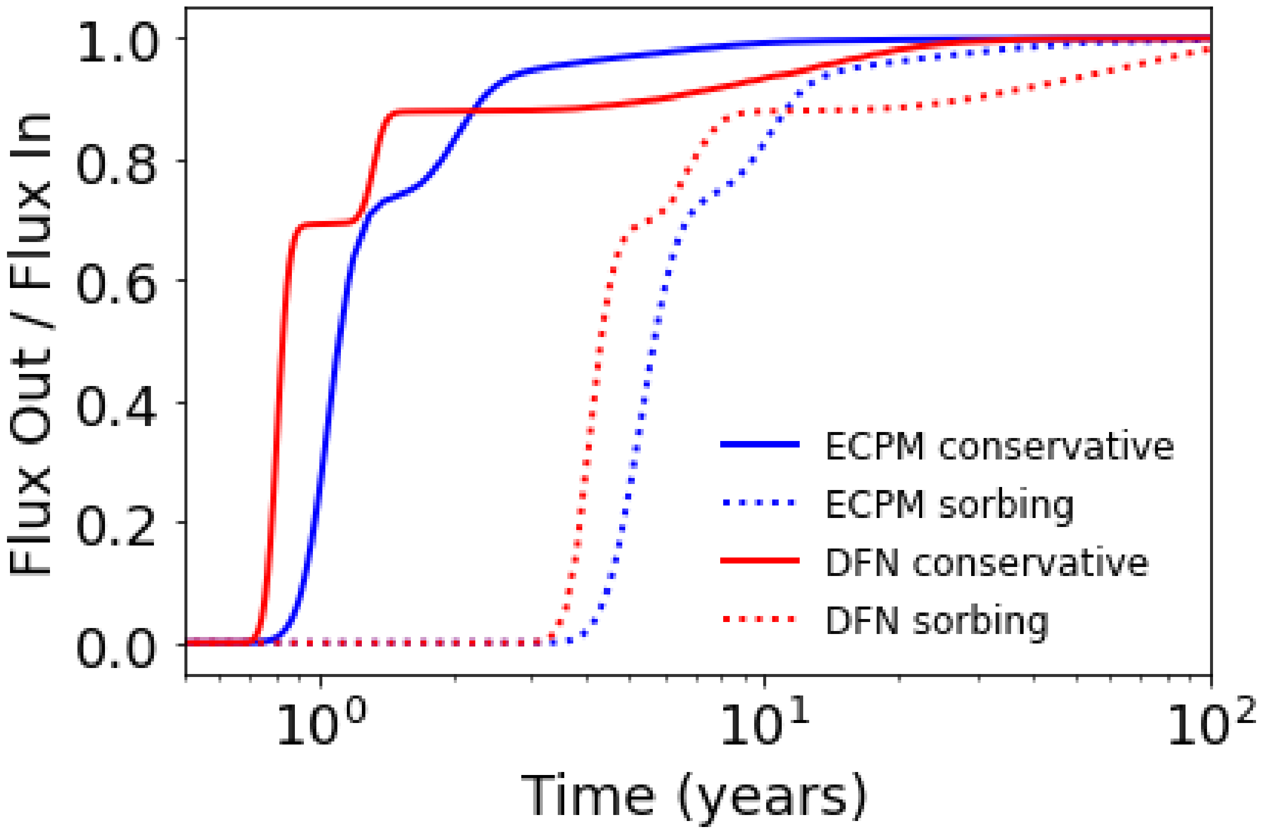
DECOVALEX Benchmark Case

- **Four deterministic fractures plus stochastic fractures**
  - Continuous point source injection
  - ECPM delays fastest 90% and speeds up slowest 10%

continuous point source

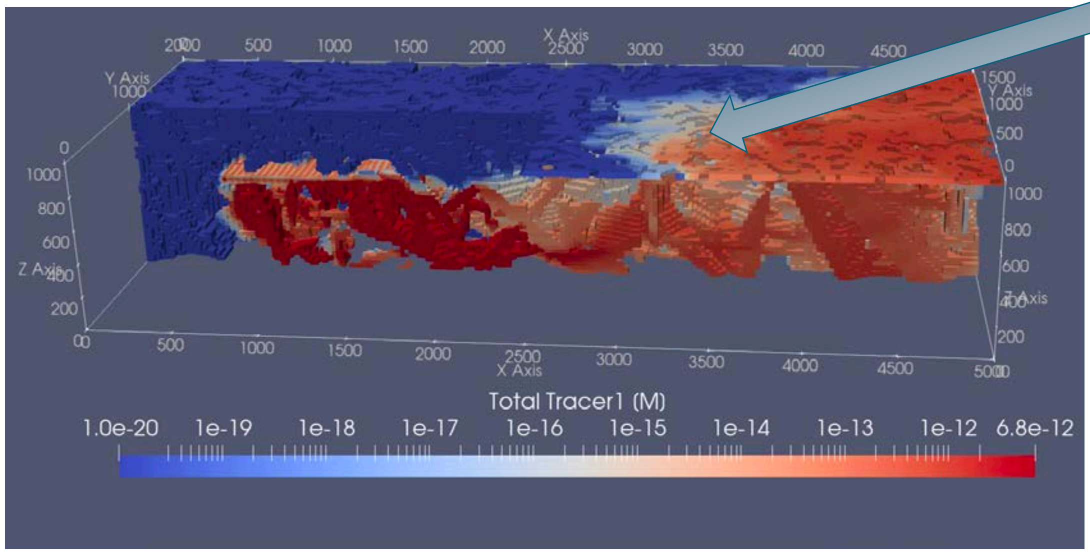


1000 m

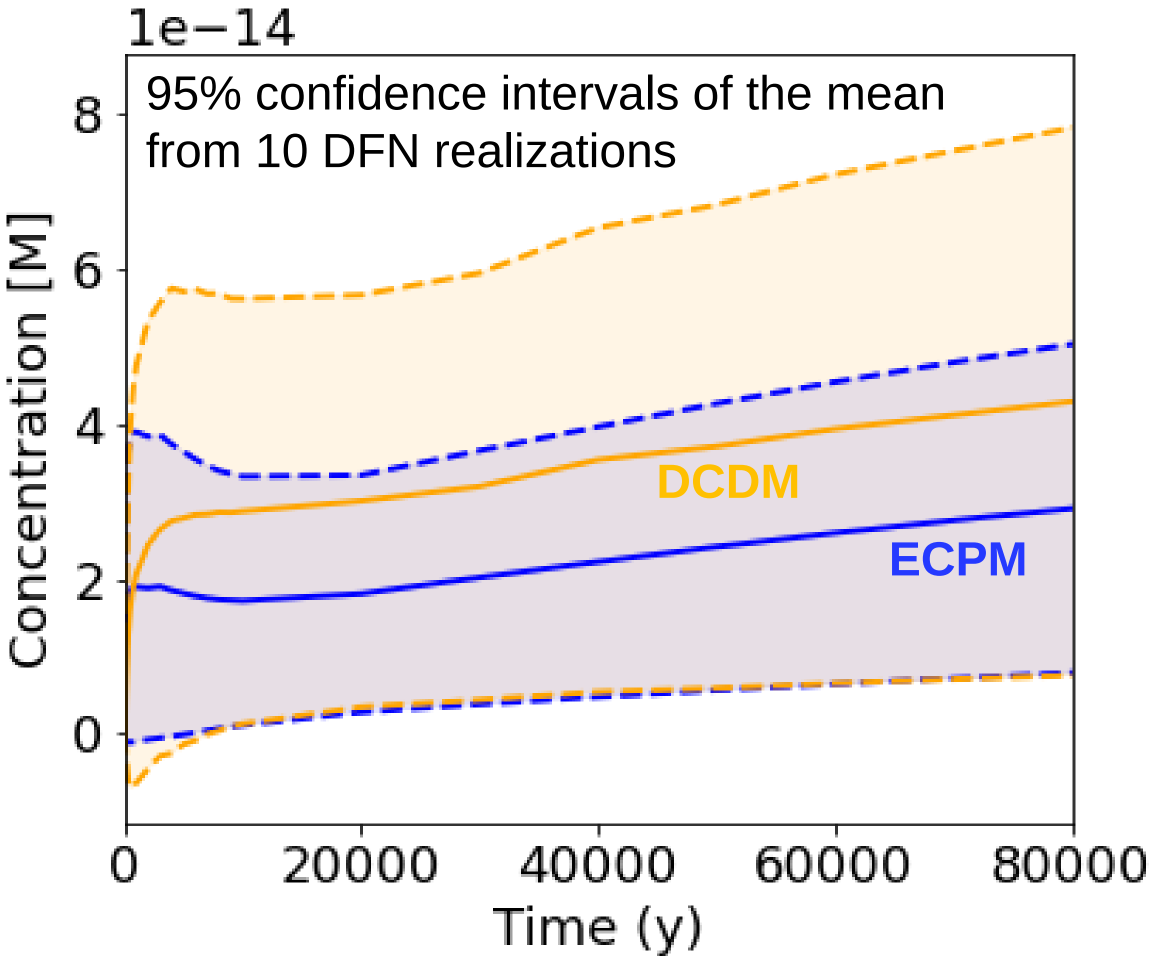


DECOVALEX Full Reference Case

- **Dual continuum (DCDM) leads to increased concentration possibly due to less numerical dispersion**



Tracer concentration at 10,000 years



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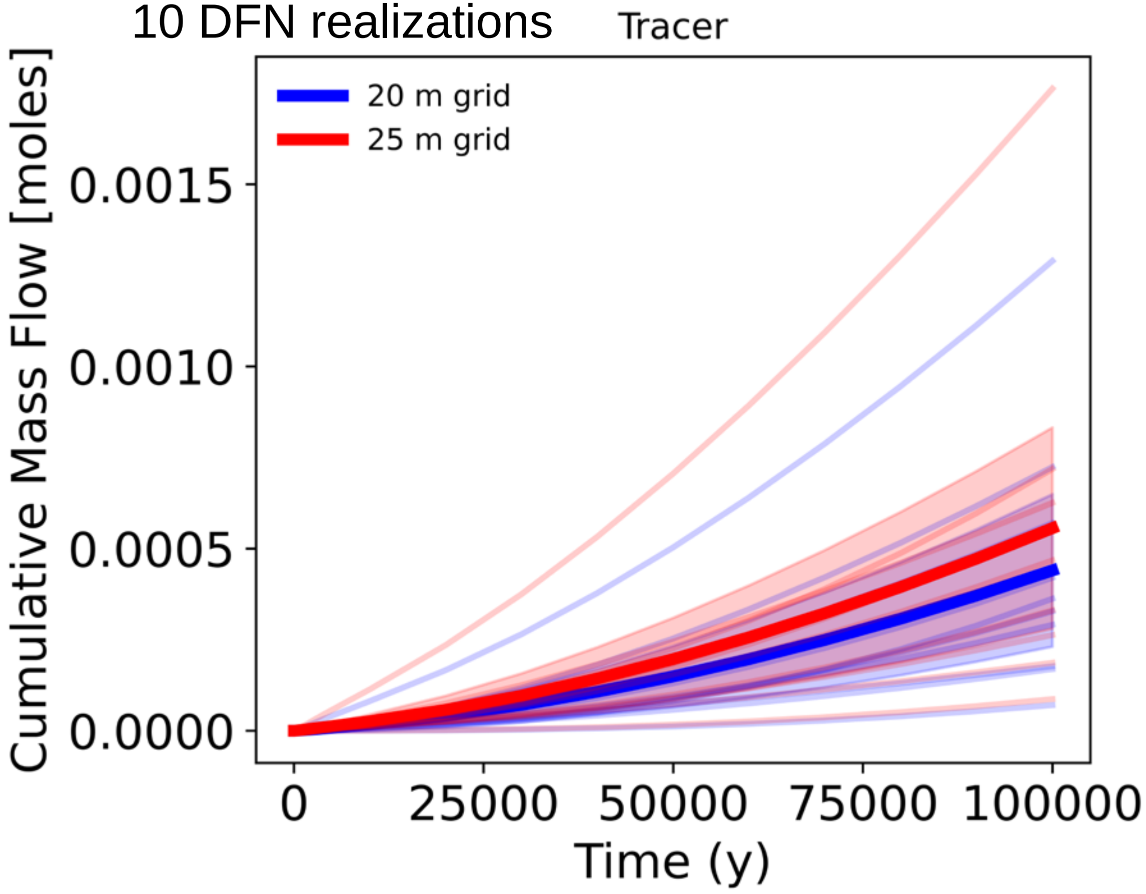
Summary of Reference Case

- **What did we learn looking at the conservative tracers?**
  - Assumptions made in repository can lead to large differences in far field observations
  - Domain scale heterogeneity plays role in far field observations
  - Choice in grid cell size can significantly reduce run times
  - Further information to be learned → project to continue on next 4 years

10 DFN realizations



Cell with maximum mass flow out of domain

Radionuclide Decay Chain in Reference Case

- **Isotope Partitioning and Decay Model**
  - Isotope partitioning among aqueous, solid, and adsorbed phases
  - Decay and ingrowth in all phases
  - Implemented in DECOVALEX reference case for ECPM and DCDM

Table 3-7 Radionuclide inventory in second iteration of reference case

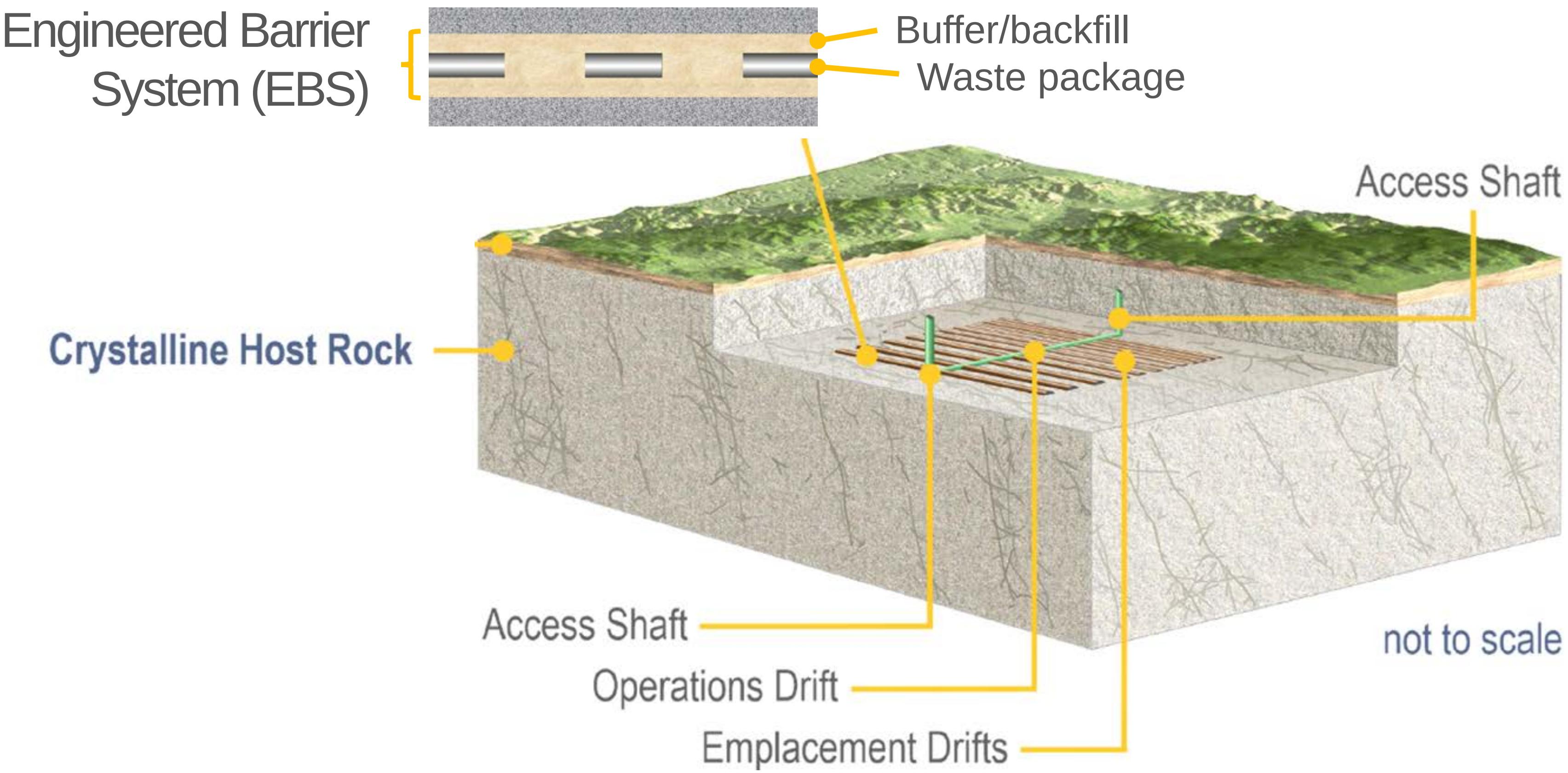
Isotope	Atomic weight (g/mole)	Inventory per waste package (g)	Decay Constant (1/yr)	Daughter	Instant Release Fraction
^{129}I	128.9	5.45E+02	4.41E-08		10%
^{226}Ra	226.03	6.94E-05	4.33E-04		0%
^{230}Th	230.03	1.81E-01	9.00E-06	^{226}Ra	0%
^{234}U	234.04	8.89E+02	2.83E-06	^{230}Th	0%
^{238}U	238.05	1.58E+06	1.55E-10	^{234}U	0%

Performance Factor Analysis

Sources of Performance

Where does performance come from?

Natural barriers & engineered barriers



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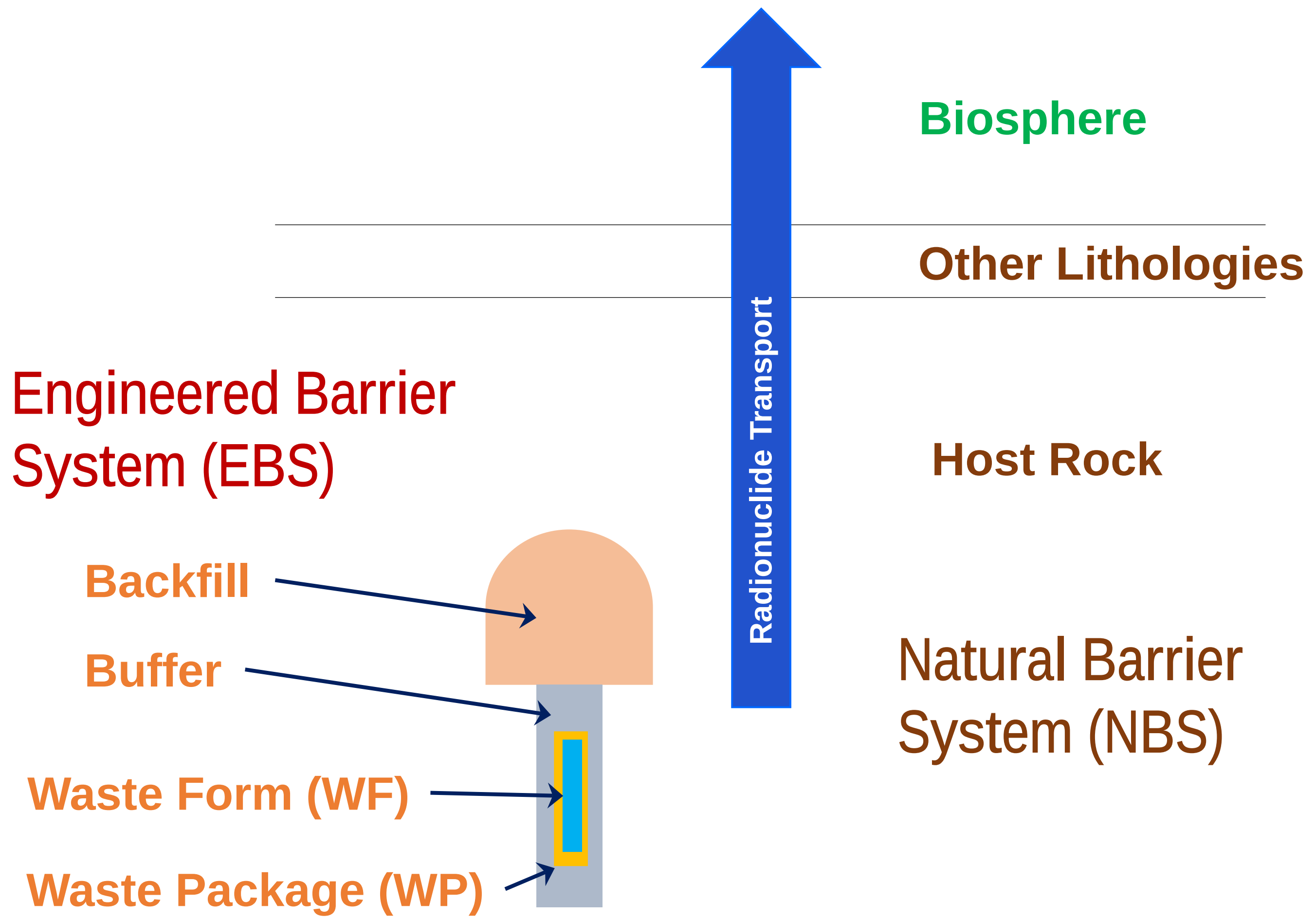
Performance of Engineered Barriers

How much performance comes from engineered barriers?

Model estimates depend on

- Repository design
- Geosphere/biosphere characteristics
- Model assumptions and simplifications



Measuring Performance

- **Performance of overall repository system**
  - Measured by calculating (probabilistically) the peak of the performance metric during the regulatory period in a full system model and comparing it to the regulatory limit
- **Performance of individual components or subsystems**
  - Measured by calculating ***performance factors*** (F_i)
- **Performance factor (F_i)**
  - Measures the factor contribution of component i to performance

$$F_i = \frac{H}{H_i}$$

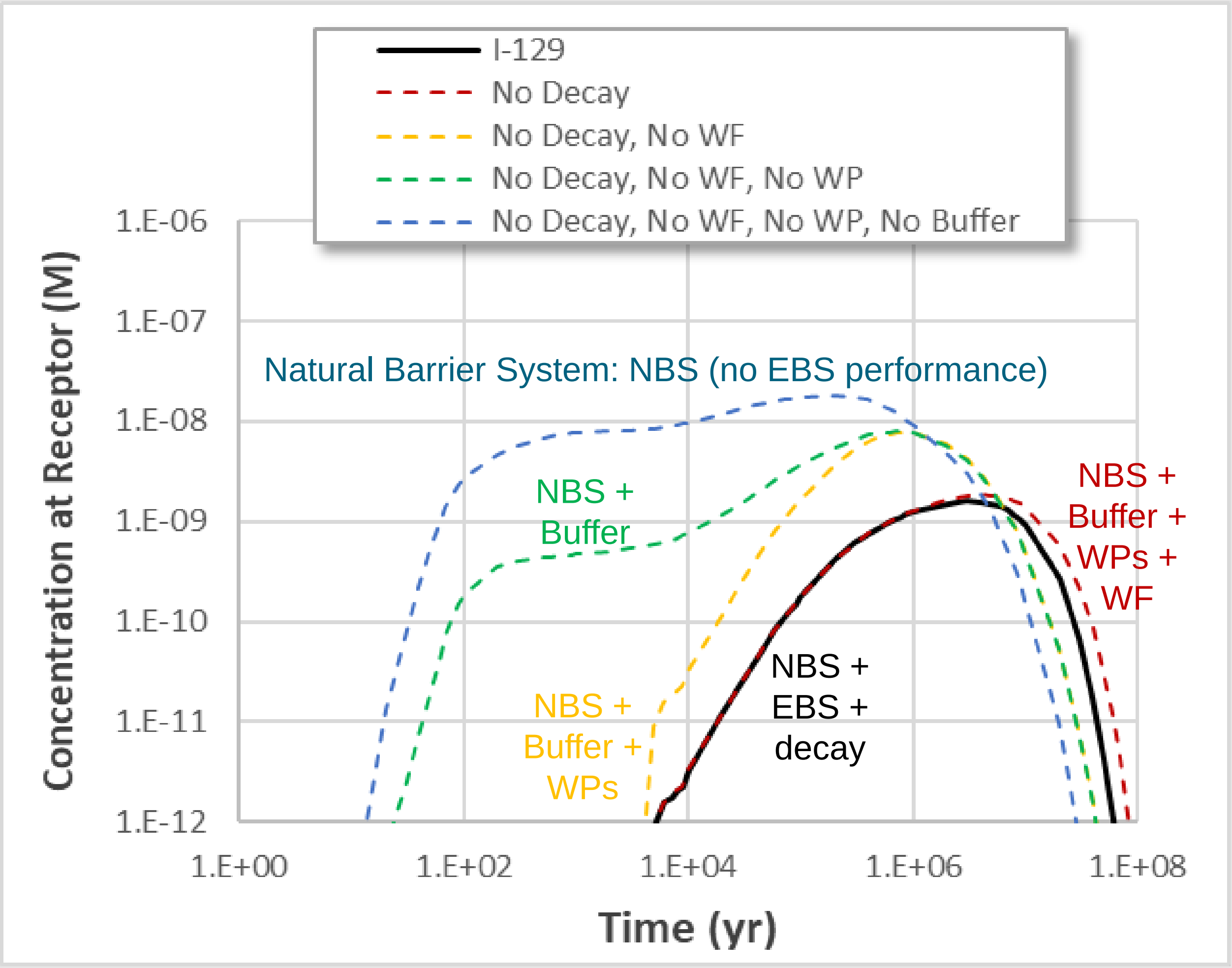
H: Value of performance metric when component i is *excluded*

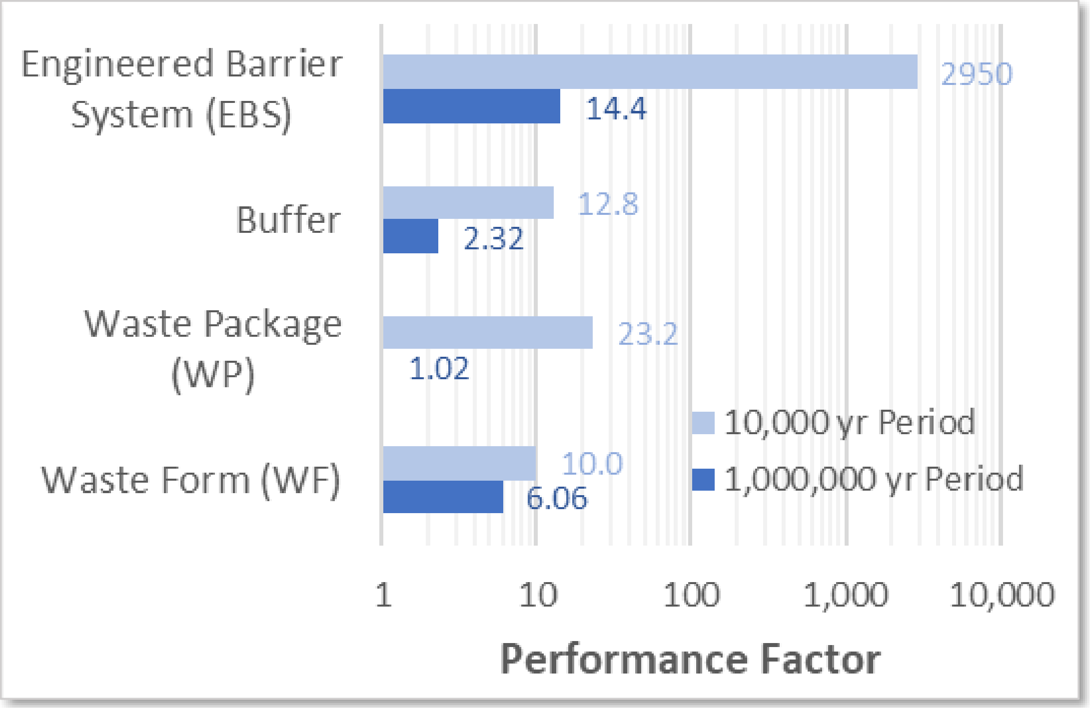
H_i: Value of performance metric when component i is *included*

For example, if the dose is 9 times higher when component i is excluded, then F_i = 9

Mariner et al. (2024)

Performance Factor Analysis for DECOVALEX Crystalline Reference Case





- **Waste packages and waste form matrix included in this DECOVALEX crystalline reference case**
- **Performance factors (in this study) are the ratios of the peak concentrations at the receptor**

Mariner et al. (2024)

Considerations for Using Performance Factors

- **Quantify/Communicate Modeled Barrier Performance Impact**
  - Evaluate changes for ranges of barrier lifetimes – planning/design feedback
  - Assess risk/benefit for modifying engineered barriers
  - Communicate differential reliance on Natural Barriers and Engineered Barriers for different generic Disposal Concept models
- **Demonstration of Multiple Barrier Performance Reliance**
  - Solubility-limited concentrations for radionuclides (throughout system)
  - Performance contributions of barriers to range of radionuclides
    - Communicate effect of the geology for many radionuclides
- **Proceed with Careful Analysis of Results**
  - Understand what the performance factor includes/excludes
  - Identify aspects of model uncertainty re: barrier performance “assumptions”
  - Investigate sensitivities

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Questions