Estimating The Effect Of Fracture Connectivity On Waste Isolation Using A High-Performance Reactive Transport Simulator, PFLOTRAN

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Problem

- **How does uncertainty in fracture inter-connectivity affect predictions of waste isolation, i.e., predictions of the rate of radionuclide transport from a high-level nuclear waste repository in a fractured host rock**
  - Fracture connectivity is determined by temperature and stress fields at the time of rock deposition/formation
  - Natural system heterogeneity will always have uncertainty associated with it, which must be represented in safety assessments
- **Two end-member simulations using *GDSA Framework*, an open-source performance assessment tool for deep geologic disposal of nuclear waste:**
  - Inter-connectivity to the surface: transport controlled by advection
  - No fracture connectivity to the surface: transport controlled by diffusion

Repository Natural Barrier System

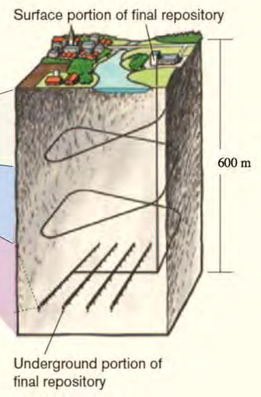
Fracture properties at Forsmark, Sweden

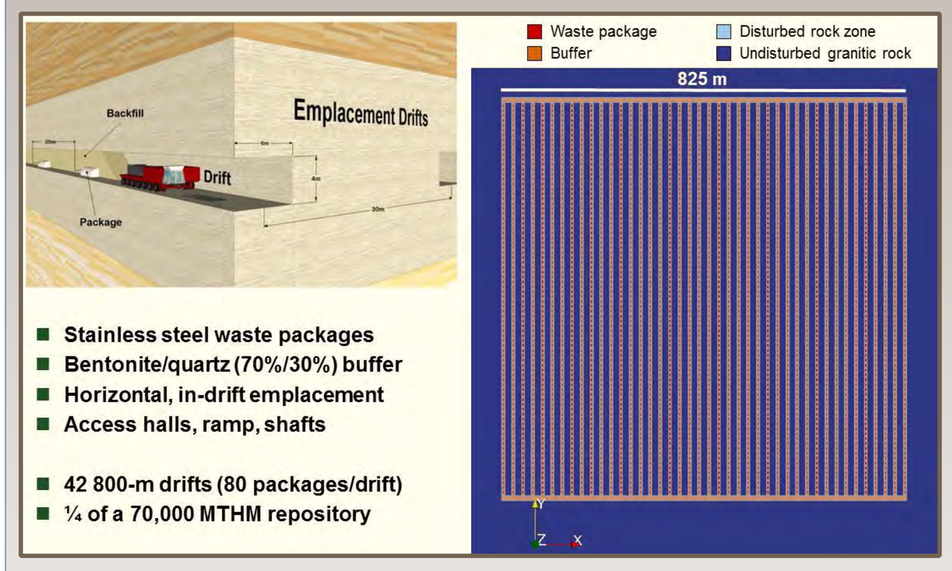
Table 2 Hydrogeological DFN parameters for each fracture domain, fracture set and depth zone

Fracture domain/elevation (m.a.s.l)[a]	Fracture set name	Orientation set pole: (trend, plunge), conc.	Size model, power-law (r_0, k_r) (m, –)	Intensity, (P_{32}), valid size interval: r_0 to 564 m (m^2/m^3)	Parameter values for the transmissivity models: Semi-correlated (a,b,σ)	Correlated (a,b)	Uncorrelated (μ,σ)
FFM01 and FFM06>–200	NS	(292, 1) 17.8	(0.038, 2.50)	0.073	$6.3 \cdot 10^{-9}$, 1.3, 1.0	$6.7 \cdot 10^{-9}$, 1.4	−6.7, 1.2
	NE	(326, 2) 14.3	(0.038, 2.70)	0.319			
	NW	(60, 6) 12.9	(0.038, 3.10)	0.107			
	EW	(15, 2) 14.0	(0.038, 3.10)	0.088			
	HZ	(5, 86) 15.2	(0.038, 2.38)	0.543			
FFM01 and FFM06 –200 to –400	NS	(292, 1) 17.8	(0.038, 2.50)	0.142	$1.3 \cdot 10^{-8}$, 0.5, 1.0	$1.6 \cdot 10^{-9}$, 0.8	−7.5, 0.8
	NE	(326, 2) 14.3	(0.038, 2.70)	0.345			
	NW	(60, 6) 12.9	(0.038, 3.10)	0.133			
	EW	(15, 2) 14.0	(0.038, 3.10)	0.081			
	HZ	(5, 86) 15.2	(0.038, 2.38)	0.316			
FFM01 and FFM06<–400	NS	(292, 1) 17.8	(0.038, 2.50)	0.094	$5.3 \cdot 10^{-11}$, 0.5, 1.0	$1.8 \cdot 10^{-10}$, 1.0	−8.8, 1.0
	NE	(326, 2) 14.3	(0.038, 2.70)	0.163			
	NW	(60, 6) 12.9	(0.038, 3.10)	0.098			
	EW	(15, 2) 14.0	(0.038, 3.10)	0.039			
	HZ	(5, 86) 15.2	(0.038, 2.38)	0.141			
FFM02>–200	NS	(83, 10) 16.9	(0.038, 2.75)	0.342	$9.0 \cdot 10^{-9}$, 0.7, 1.0	$5.0 \cdot 10^{-9}$, 1.2	−7.1, 1.1
	NE	(143, 9) 11.7	(0.038, 2.62)	0.752			
	NW	(51, 15) 12.1	(0.038, 3.20)	0.335			
	EW	(12, 0) 13.3	(0.038, 3.40)	0.156			
	HZ	(71, 87) 20.4	(0.038, 2.58)	1.582			
FFM03, FFM04 and FFM05>–400	NS	(292, 1) 17.8	(0.038, 2.60)	0.091	$1.3 \cdot 10^{-8}$, 0.4, 0.8	$1.4 \cdot 10^{-8}$, 0.6	−7.2, 0.8
	NE	(326, 2) 14.3	(0.038, 2.50)	0.253			
	NW	(60, 6) 12.9	(0.038, 2.55)	0.258			
	EW	(15, 2) 14.0	(0.038, 2.40)	0.097			
	HZ	(5, 86) 15.2	(0.038, 2.55)	0.397			
FFM03, FFM04 and FFM05<–400	NS	(292, 1) 17.8	(0.038, 2.60)	0.102	$1.8 \cdot 10^{-8}$, 0.3, 0.5	$7.1 \cdot 10^{-9}$, 0.6	−7.2, 0.8
	NE	(326, 2) 14.3	(0.038, 2.50)	0.247			
	NW	(60, 6) 12.9	(0.038, 2.55)	0.103			
	EW	(15, 2) 14.0	(0.038, 2.40)	0.068			
	HZ	(5, 86) 15.2	(0.038, 2.55)	0.250			

[a] Meters above sea level

Joyce et al., Hydrogeology Journal (2014) 22:1233-1249



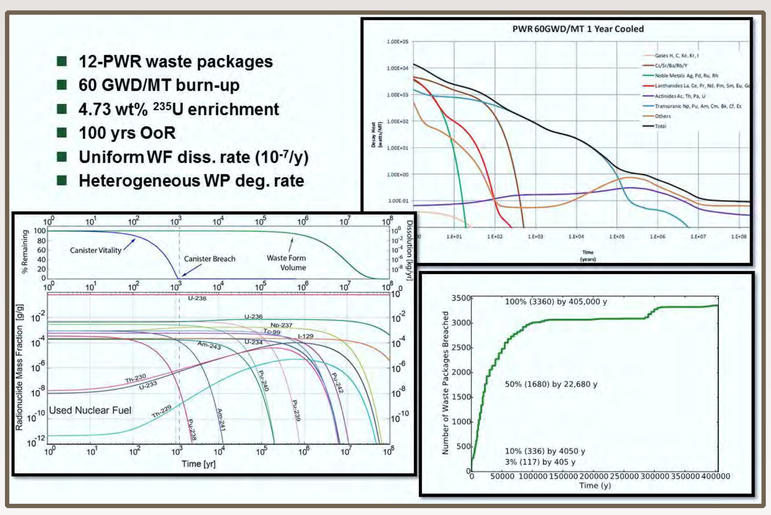


- Stainless steel waste packages
- Bentonite/quartz (70%/30%) buffer
- Horizontal, in-drift emplacement
- Access halls, ramp, shafts
- 42 800-m drifts (80 packages/drift)
- ¼ of a 70,000 MTHM repository

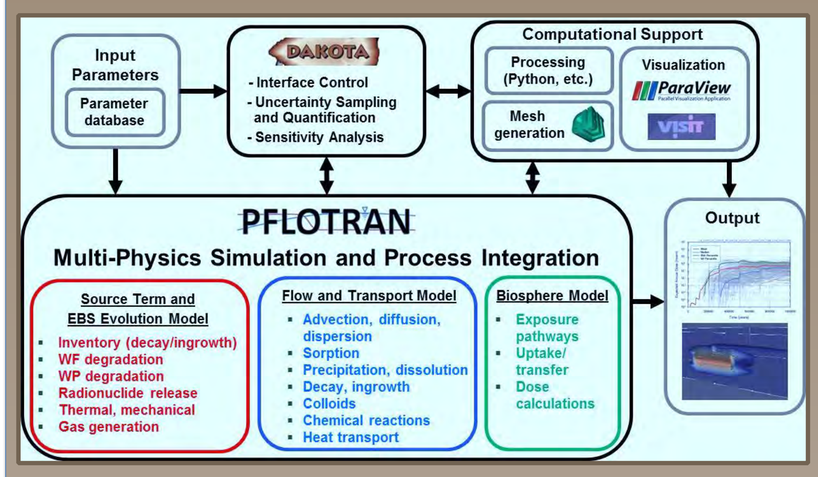
Repository Engineered Barrier System

Inventory, Decay Heat, Waste Form and Package Degradation

- 12-PWR waste packages
- 60 GWD/MT burn-up
- 4.73 wt% ^{235}U enrichment
- 100 yrs OoR
- Uniform WF diss. rate (10^{-7}/y)
- Heterogeneous WP deg. rate



GDSA (Geologic Disposal Safety Assessment) Framework, http://pa.sandia.gov

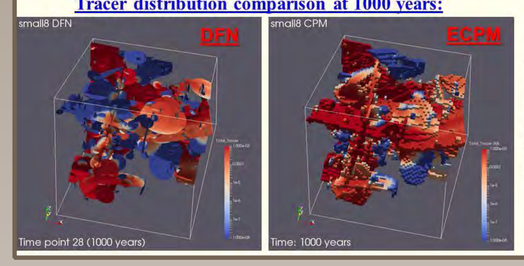


- **Domain Size:** 3015m x 2025m x 1260m
- **Cell Resolution:** 15m down to 1.67m
- **Number of Grid Cells:** 4,848,260
- **Processors Used:** 512
- **Number of Waste Forms:** 3,360
- **Real Time to Run 10^6 years:** 8 hours

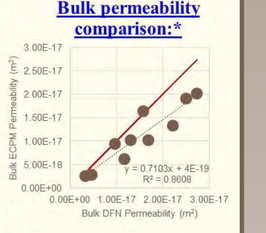
Conceptual and Numerical Considerations

- **Discrete fracture networks (DFNs), commonly used to model isothermal fluid flow and radionuclide transport in fractured rock, do not include the effects of heat on fluid flow**
- ***GDSA Framework* has mapped a DFN (generated with dfnWorks) to an equivalent continuous porous medium (ECPM) in PFLOTRAN**
  - Determines which ECPM 3-D grid cells are intersected by DFN fracture planes
  - Adjusts anisotropic permeability and porosity of ECPM "fracture cells" to represent those same properties of the DFN

Tracer distribution comparison at 1000 years:



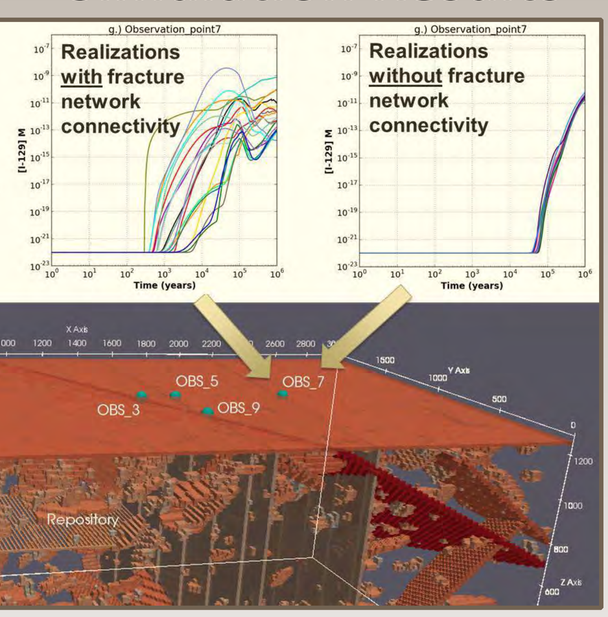
Bulk permeability comparison:*



* Stein et al. 2017 (at IHLRWM 2017 in Charlotte)

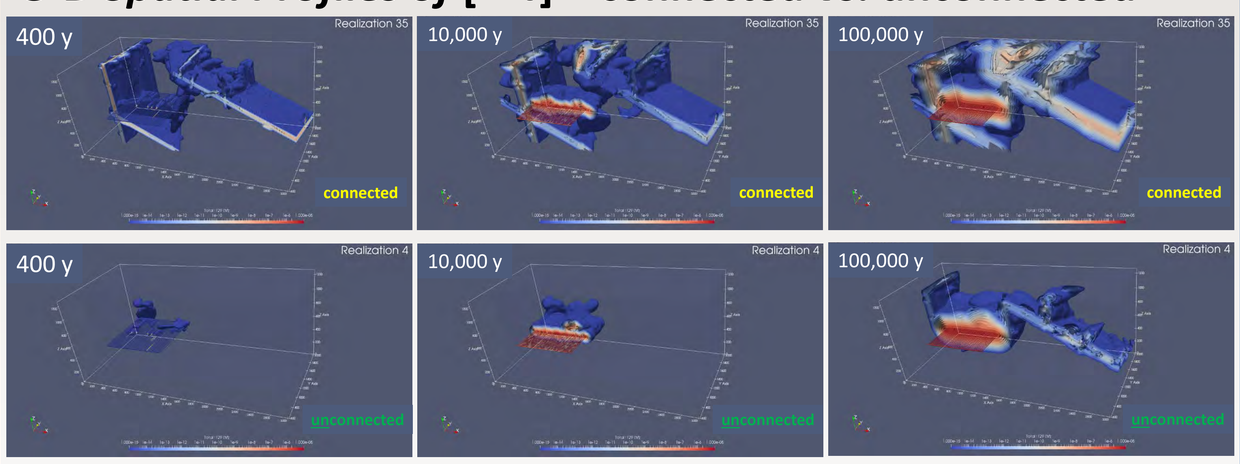
Simulation Results

- Observation points are within the 15 m thick sedimentary overburden
- The repository is about 600 m below the sediment

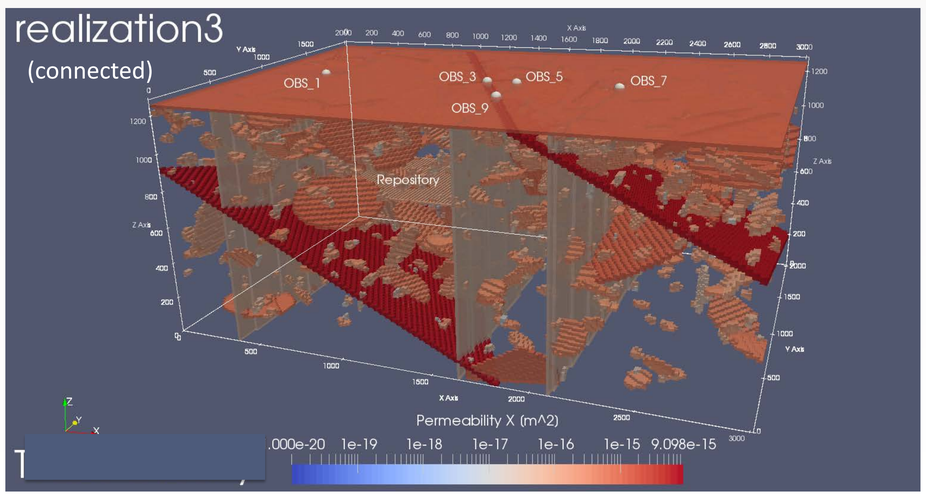


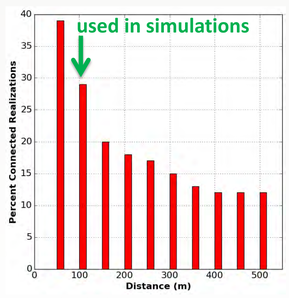
Time Histories of ^{129}I Breakthrough at the Surface

3-D Spatial Profiles of [^{129}I] – connected vs. unconnected



Repository Layout & Simulation Domain





Probability of Fracture Connectivity to the Surface as a Function of Distance of Nearest Vertical Feature to the Repository

Conclusions & Future Work

- For deep geologic repositories in fractured host rock, sufficient site-specific understanding of deterministic features and of the probability of a percolating fracture network will provide confidence in the operation of the waste isolation safety function
- *GDSA Framework* (pa.sandia.gov) provides the open-source computational and modeling capability to investigate coupled processes of heat flow, buoyant two-phase fluid flow, and radionuclide transport in a large 3-D spatially heterogeneous permeable rock domain
- The effect of multiple input uncertainties (spatial variability combined with multiple property uncertainties) will be examined through multi-realization simulations and sensitivity analyses

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