Advances in Sensitivity Analysis for the Crystalline Reference Case

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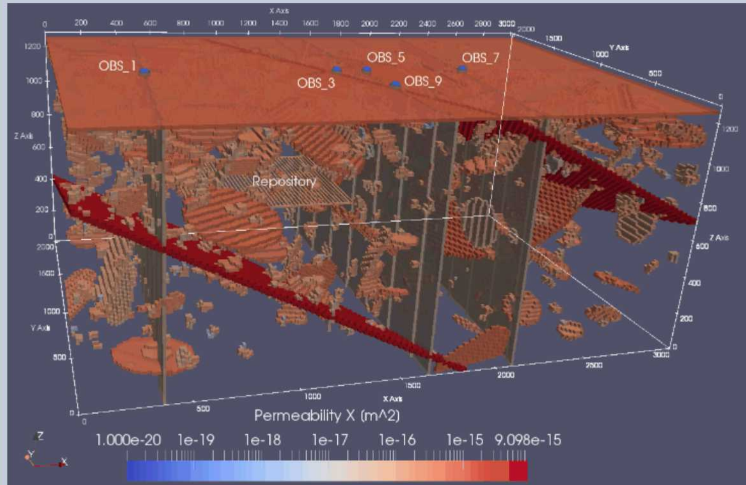


OBJECTIVE

To perform crystalline reference case sensitivity analyses to study the relative importance of uncertain parameters on peak concentration and breakthrough time in overlying sediments

- WP degradation rate distribution mean and standard deviation
- Waste form dissolution rate
- Permeabilities (buffer, DRZ, overlying aquifer)
- Buffer porosity
- Future
  - WP degradation rate spatial assignments order (among WPs)
  - Discrete fracture network (DFN) realization

CRYSTALLINE REFERENCE CASE

Computational Requirements:

- **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 Gridded Waste Forms:** 3,360
- **Real Time to Run 10^6 years:** ~7.5 hrs (50y Max Timestep), ~7 hrs (500y Max Timestep), ~1.5 hrs (5,000y Max Timestep)

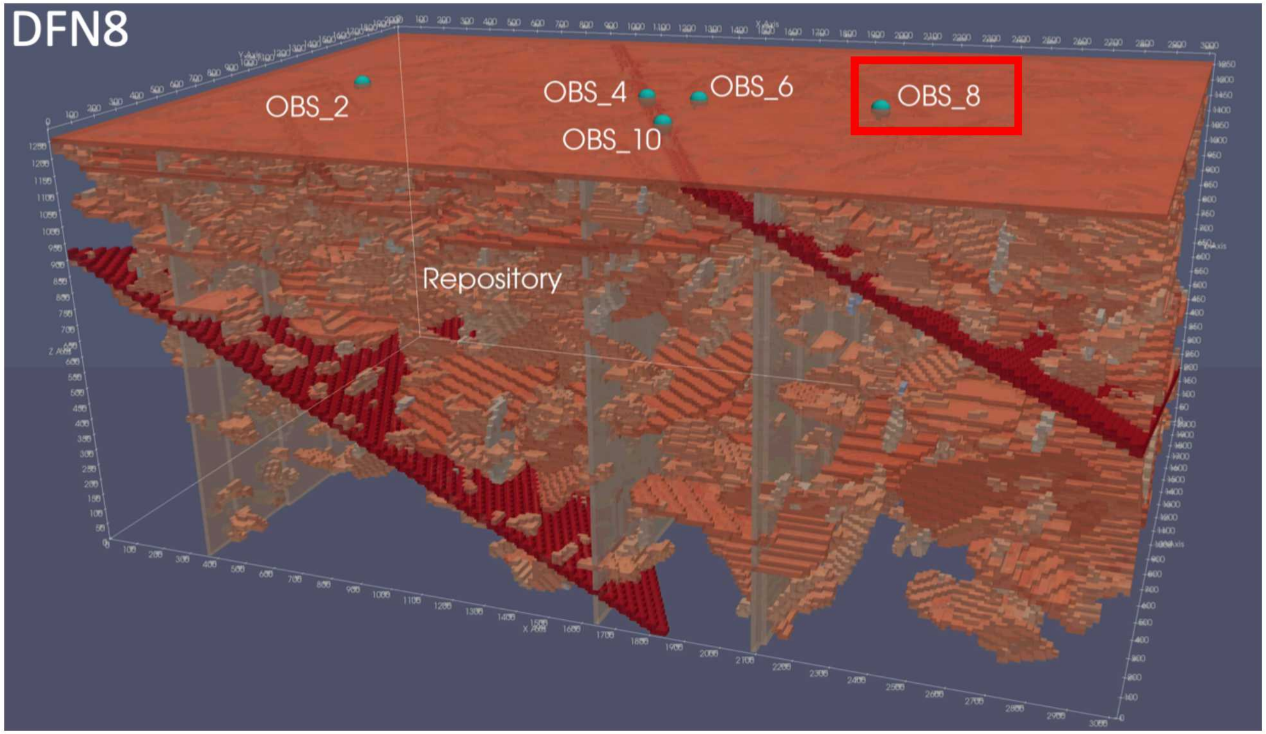


Figure. DFN 8 realization mapped to porous medium grid, showing the model domain and location of the repository. Fractures of the DFN realization are shown in orange. Unconnected fractures are removed. Five deterministic fracture zones, three sub-vertical (gray) and two with a dip of approximately 30 degrees (red), are common to each DFN realization. Observation points are located above the midline of the repository where the deterministic fracture zones intersect the top boundary.

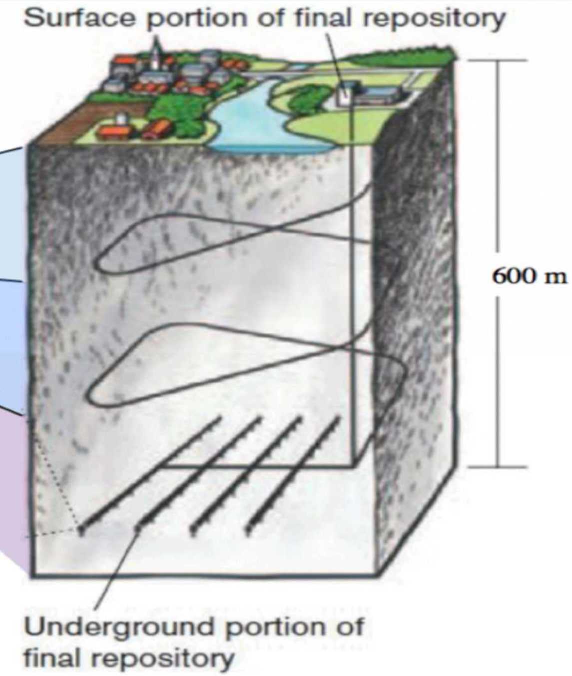
- **Waste Package (WP):** Stainless steel canister containing 12 PWR UNF assemblies (5.22 MTHM) and stainless steel overpack.

DFN Generation

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	$1.3 \cdot 10^{-9}$, 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



- dfnWorks was used to generate 30 DFNs over three layers of decreasing fracture density with depth
- All 30 DFNs are considered aleatory because they are randomly generated
- DFN 8 was selected for all epistemic analysis, due to its average breakthrough times at certain observation points

Sensitivity Analyses

A. Sensitivity analysis to look at the effect of variance in the spatial distribution of WP degradation rate on peak concentration and breakthrough times

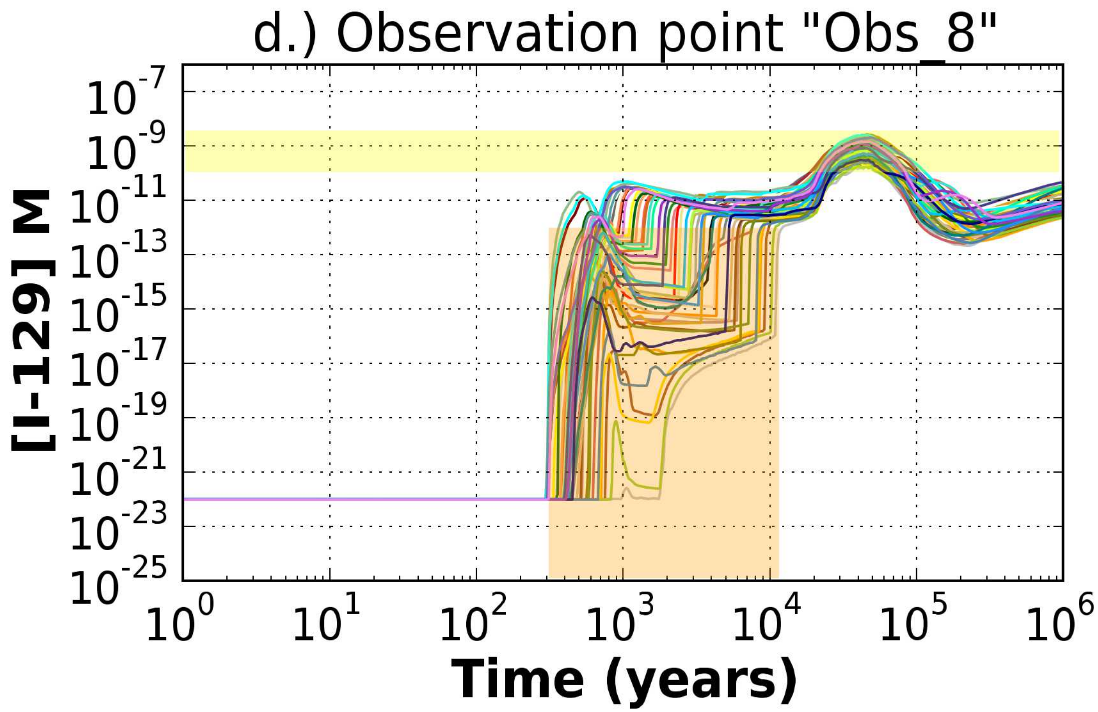
B. Sensitivity analysis of epistemic uncertainties (and maximum time step size) on peak concentration and breakthrough times

C. Future: Sensitivity analysis that includes both aleatory and epistemic uncertainties

Parameter	Lower Bound	Upper Bound	Distribution
Used nuclear fuel (UNF) fractional dissolution rate (rateUNF) (yr^{-1})	10^{-8}	10^{-6}	Log uniform
Glacial permeability (kGlacial) (m^2)	10^{-16}	10^{-13}	Log uniform
Damaged rock zone (DRZ) permeability (permDRZ) (m^2)	10^{-19}	10^{-16}	Log uniform
Buffer permeability (permBuffer) (m^2)	10^{-20}	10^{-17}	Log uniform
Buffer porosity (pBuffer)	0.3	0.5	Uniform
Log of mean waste package fractional degradation rate at 60°C (rateWP) (yr^{-1}) *	-5.5	-4.5	Uniform
Standard deviation of the sampled mean log rate (stdWPrate)	0	0.5	Uniform

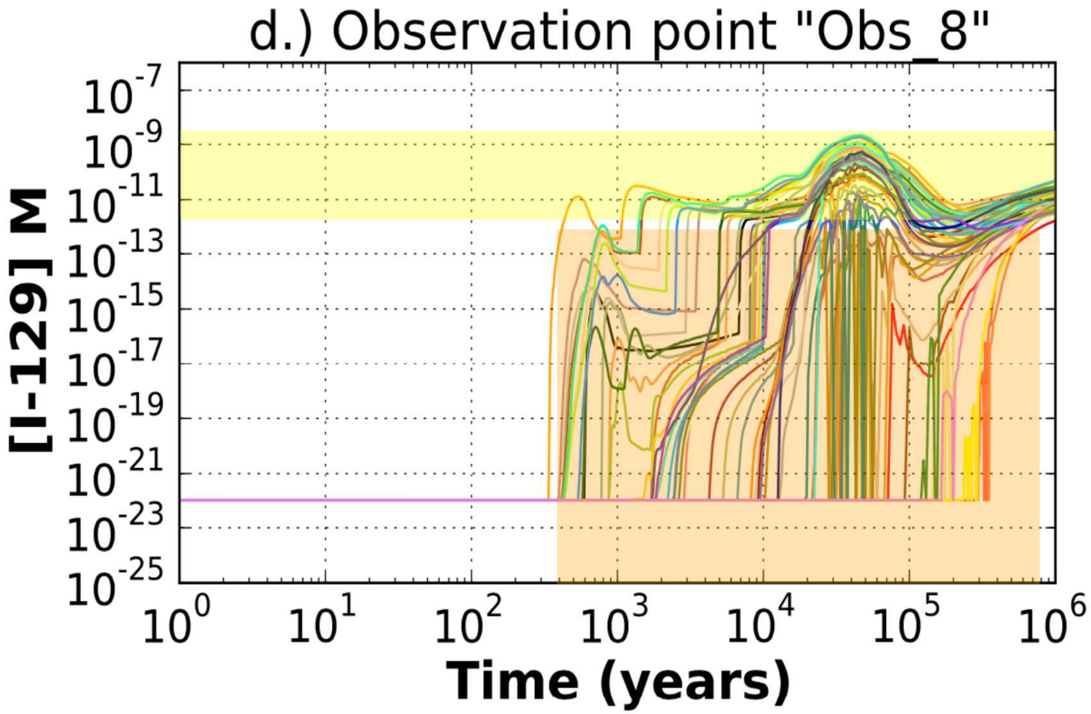
Sensitivity Analysis A: stdWPrate of 0.5

- Same DFN, max timestep size, and order of WP degradation rate assignments
- Standard deviation waste package degradation rate (stdWPrate) set to 0.5



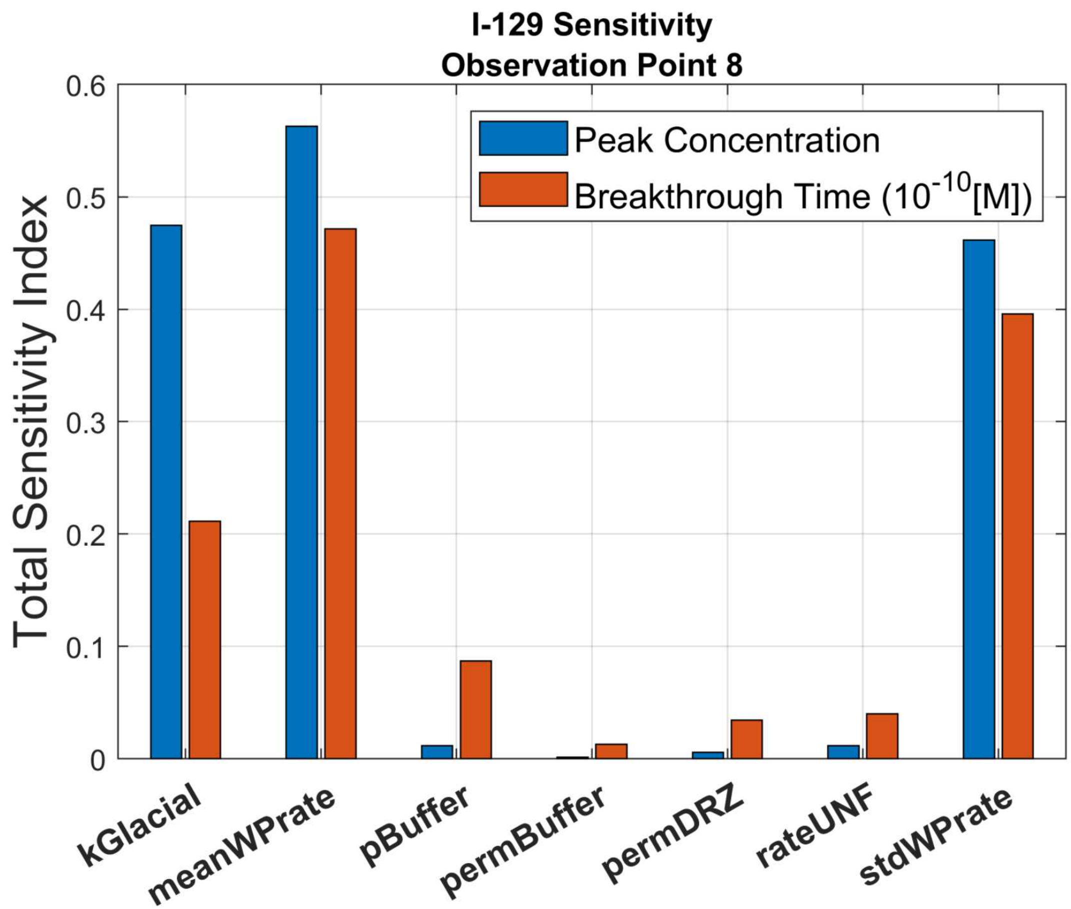
Sensitivity Analysis A: stdWPrate Varied Between 0 and 0.5

- Same DFN, max timestep size, and order of WP degradation rate assignments
- Standard deviation waste package degradation rate (stdWPrate) <u>varied between 0 and 0.5</u>
- Maximum peak concentration over all realizations is the same but uncertainty in peak concentration is increased by varying stdWPrate
- Breakthrough times are highly sensitive to stdWPrate



Sensitivity Analysis B – Epistemic Uncertainty (Granite)

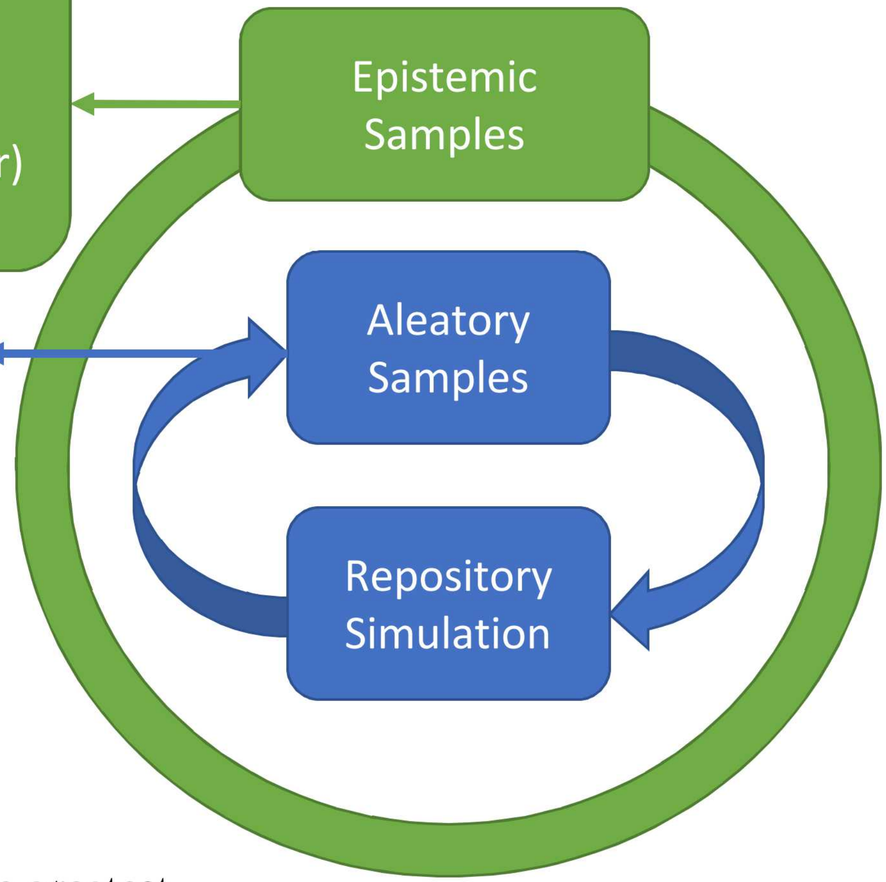
- Only epistemic uncertainty
  - Single loop
  - 7 uncertain inputs, 200 realizations
- kGlacial, meanWPrate and stdWPrate are the most important parameters
- Peak concentration is sensitive to kGlacial but breakthrough time is not
- I-129 concentration and breakthrough time are highly sensitive to uncertainty in WP degradation rate distribution mean and standard deviation



Future Analysis – Consider mixed uncertainties using nested sampling

- WP degradation rate distribution mean and standard deviation
- Waste form dissolution rate
- Permeabilities (buffer, DRZ, overlying aquifer)
- Buffer Porosity

- Discrete fracture network (DFN) realization
- WP degradation rate spatial assignments order (among WPs)



- Each epistemic sample (WP degradation rate distribution mean and standard deviation, dissolution rate, permeability, porosity) is used for each aleatory sample (DFN and WP rate spatial assignment)
- Results will inform which uncertainties have the greatest effect on I-129 peak concentration and breakthrough time

CONCLUSIONS

- Uncertainty in the waste package degradation rate distribution is an important driver of uncertainty in peak iodine concentration and breakthrough time in overlying sediments
- Future work will assess how this effect compares to the effects of the DFN realization and waste package degradation rate spatial assignment order among WPs

Questions?

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Backup Slides

CRYSTALLINE REFERENCE CASE

Drift seal length (m)	10	5
Drift length, including seals (m)	805	805
Shaft access diameter (m)	5.4	NA
Access hall/ramp height (m)	5	5
Access hall/ramp width (m)	8	8.35
Number of drifts	168	42
Number of access halls	1	2
Repository		
Number of drift pairs (rounded up)	84	NA
Repository length (m)	1,618	822
Repository width (m)	1,665	825
Repository Depth (m)	600	585

Table 4-2. PWR UNF inventory of selected radionuclides for the crystalline reference case.

Isotope	Inventory (g/MTIHM)[1]	Inventory (g/g waste)[2]	Atomic weight (g/mol)[3]	Approximate Decay Constant (1/s)
^{129}I	3.13E+02	2.17E-04	128.9	1.29E-15

[1] from Carter et al. (2013, Table C-2)
[2](g isotope/g waste) = (g isotope/MTIHM)/(g waste/MTIHM), where g waste = g all isotopes
[3]Weast and Astle (1981)

Waste Package Degradation Rate

Parameters Used to Generate DFNs

Table. Parameters used to generate discrete fracture networks.

	Set:	NS	EW	HZ
Orientation: Fisher distribution for poles	Mean Trend	90°	180°	0.0°
	Mean Plunge	0.0°	90.0°	360°
	κ	22	22	10
Size: Truncated Power Law for Radii	α	2.5	2.7	2.4
	Min Radius r_0 (m)	30	30	30
	Max Radius r_x (m)	500	500	500
Fracture Density (Requested)	Number of fractures in 1 km^3	3266	2373	5000