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Spent Fuel and Waste Science and Technology

Deep Borehole Disposal (DBD) Performance Assessment (PA) Modeling

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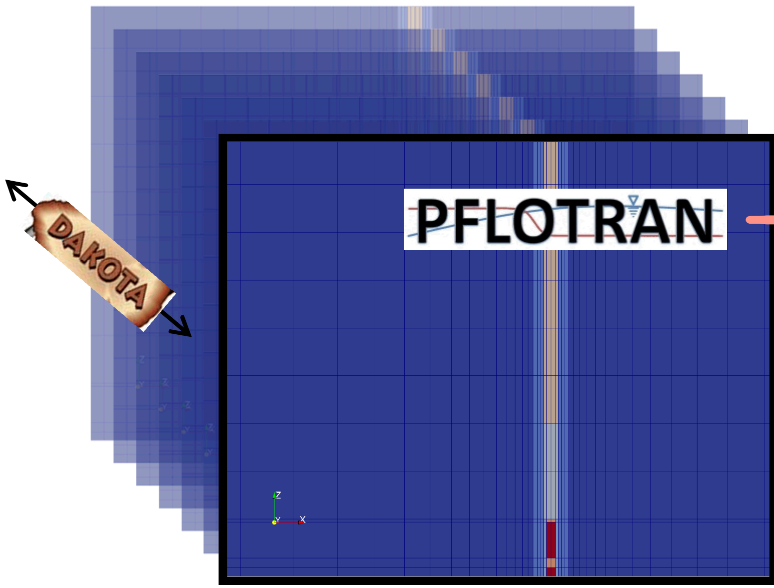
Postclosure PA Modeling

PFLOTRAN Simulations

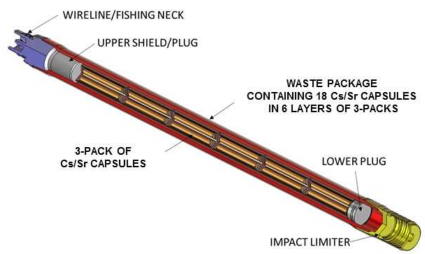


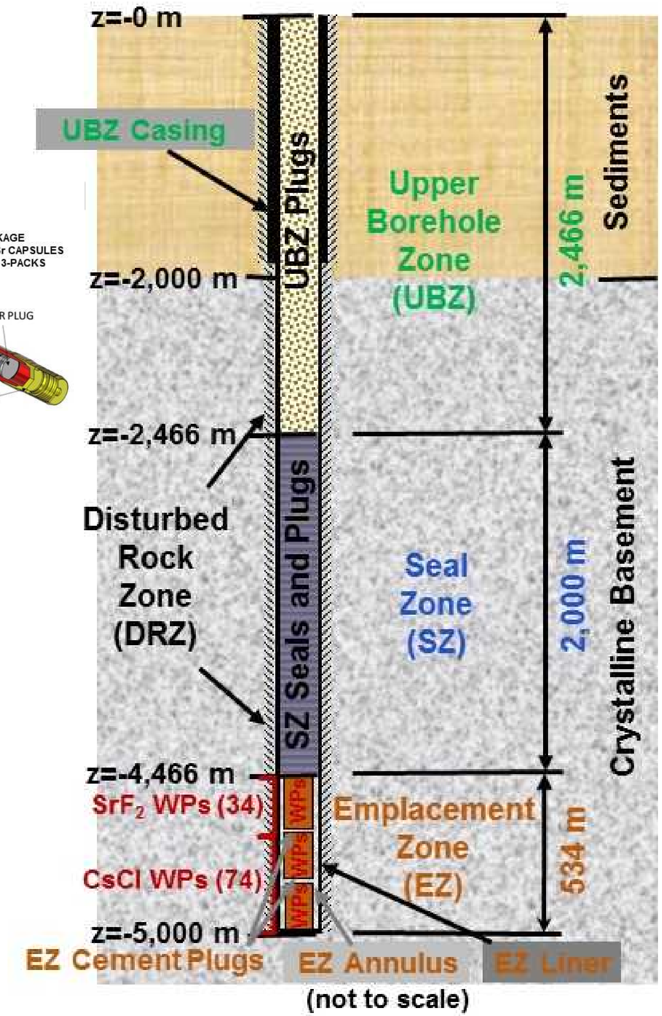
- •Coupled heat and fluid flow
- •Waste package degradation
- •Waste form dissolution
- •Radioactive decay and ingrowth
- •Solubility, sorption
- •Advection, dispersion, diffusion

- Nominal Scenario
  - *Deterministic and Probabilistic*
- Disturbed Scenario (Stuck Package)
  - *Deterministic*

Deep Borehole Disposal of Cs/Sr Capsules – Reference Design

- **1936 Cs and Sr capsules / 108 WPs**
  - 18 capsules per Waste Package (WP)
    - 6 layers of "3-packs"
    - Aged to 2050 (Freeze et al. 2016)
  - **SrF_2 : 601 capsules, ~34 WPs**
    - ^{90}Sr (1,370 g/WP)
    - 1,229 W/WP avg. thermal output
  - **CsCl: 1335 capsules, ~74 WPs**
    - ^{137}Cs (2,340 g/WP), ^{135}Cs (4,408 g/WP)
    - 978 W/WP avg. thermal output
- **All 108 WPs fit in a single borehole with an EZ (bottom-hole) diameter of 31 cm (12.25 in)**
- **Emplacement Zone Performance**
  - WP breach occurs 1 year after emplacement
  - Waste form degradation is instantaneous following WP breach
  - Unlimited radionuclide solubility





Deep Borehole Disposal of Cs/Sr Capsules – Reference Design

Seal Zone

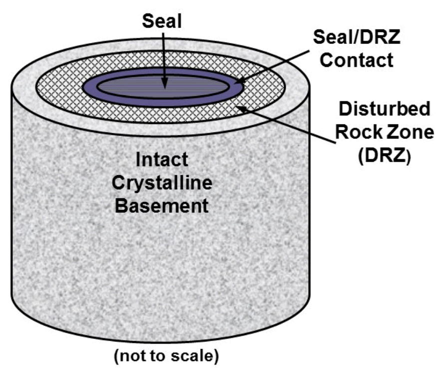
- Entirely within crystalline basement
- Seals and plugs emplaced directly against borehole wall
- Alternating sequence of materials
  - bentonite seals
  - cement plugs
  - ballast (silica sand/crushed rock)

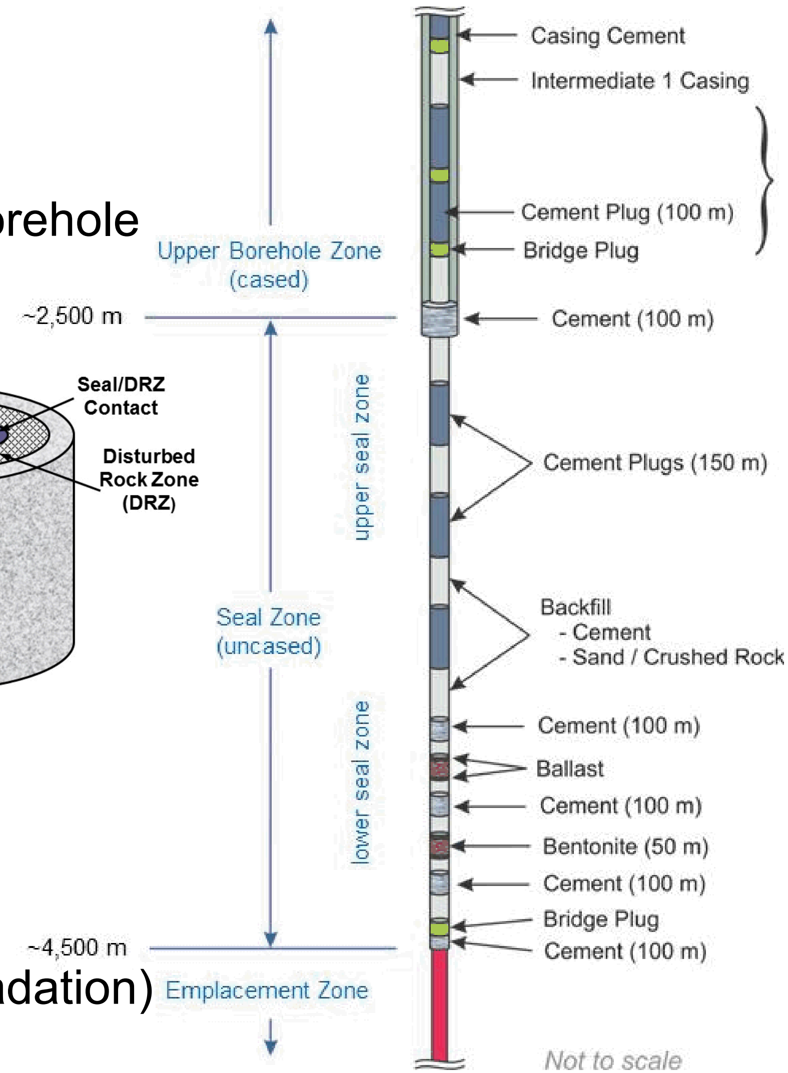
Upper Borehole Zone

- Primarily within sediments
- Plugs emplaced against cemented casing
  - cement and cement plugs

Seal Zone Performance

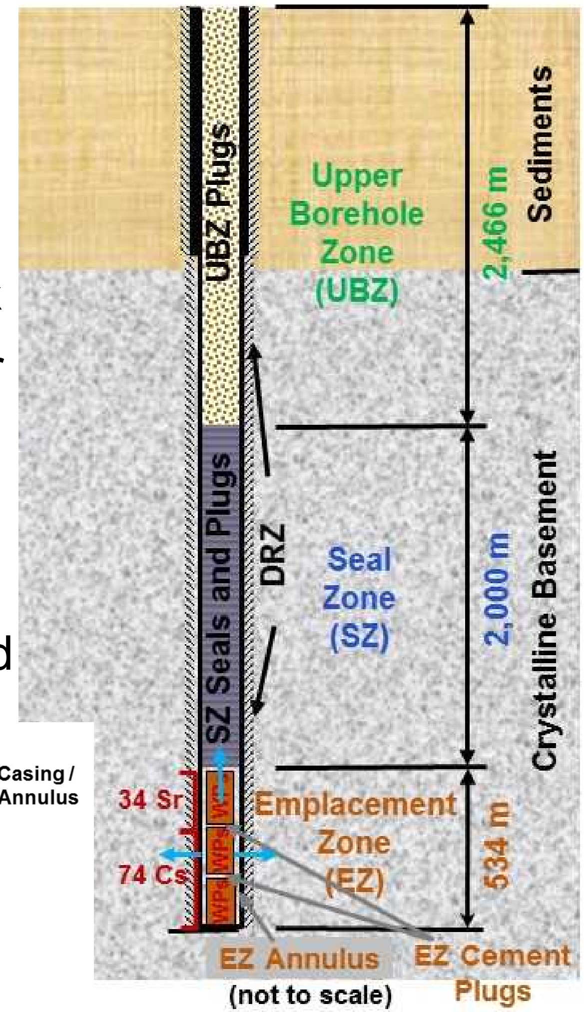
- Seal materials maintain integrity (some degradation) over period of thermally-induced upward flow

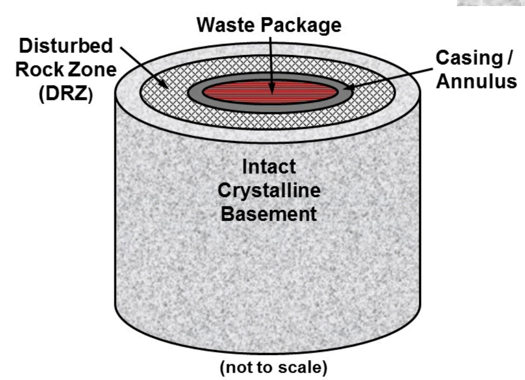




Post-Closure PA – Nominal Scenario

- **Emplacement Zone**
  - Decay heat effects:
    - Thermal perturbation in borehole produces thermally-driven upward groundwater flow
    - Heat conduction in surrounding crystalline basement rock
  - Radionuclide dissolution and transport in groundwater
    - Advection, diffusion, and decay (no sorption in EZ)
- **Post-Closure Release Pathways**
  - Radionuclide transport in groundwater by advection (thermally-induced upward flux), diffusion (upward and lateral), sorption, and decay
    - Up borehole through seals / DRZ
    - To host rock surrounding EZ
      - No regional flow gradient in crystalline basement
  - Biosphere (dose)





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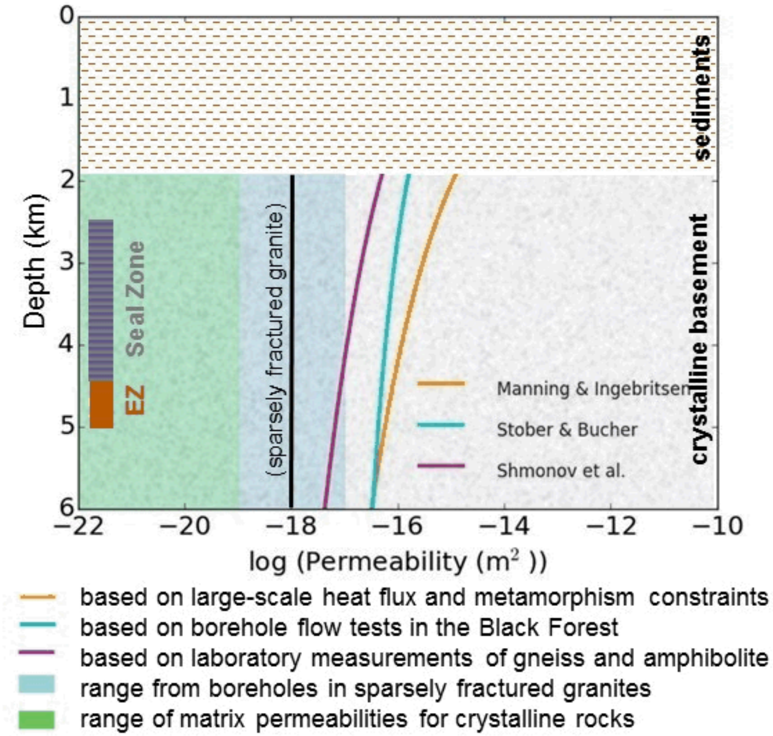
Post-Closure PA – Nominal Scenario

- **Sediments**
  - Hypothetical alternating horizontal units
- **Crystalline Basement**
  - Sparsely fractured granite
  - Heat flux = 60 W/m^2 at 6000 m
    - Thermal gradient ~ 25°C/km
    - Ambient temperature
      - 10°C at surface
      - ~125° to 140°C in EZ
  - Reducing geochemical conditions at depth
  - Salinity-dependent density gradients

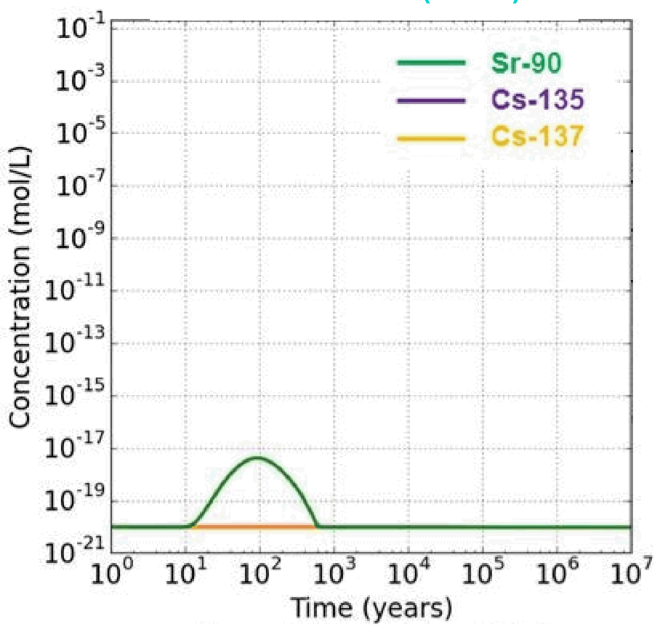


Material	Perm. (m^2)	Porosity (-)	Diffusion Coeff. (m^2/s)	Thermal Cond. (W/m·K)	Heat Capacity (J/kg·K)	Sr K_d (ml/g)	Cs K_d (ml/g)
EZ Annulus	1×10^{-12}	0.99	9.9×10^{-10}	0.58	4192	0	0
Cement Plug	1×10^{-18}	0.175	3.1×10^{-11}	1.7	900	0	0
Bentonite Seal	1×10^{-18}	0.45	2.0×10^{-10}	1.3	800	1525	560
Ballast	1×10^{-14}	0.20	4.0×10^{-11}	2.0	800	0	0
Crystalline Rock	1×10^{-18}	0.005	1.0×10^{-12}	2.5	880	1.7	22.5
DRZ	1×10^{-16}	0.005	1.0×10^{-12}	2.5	880	1.7	22.5

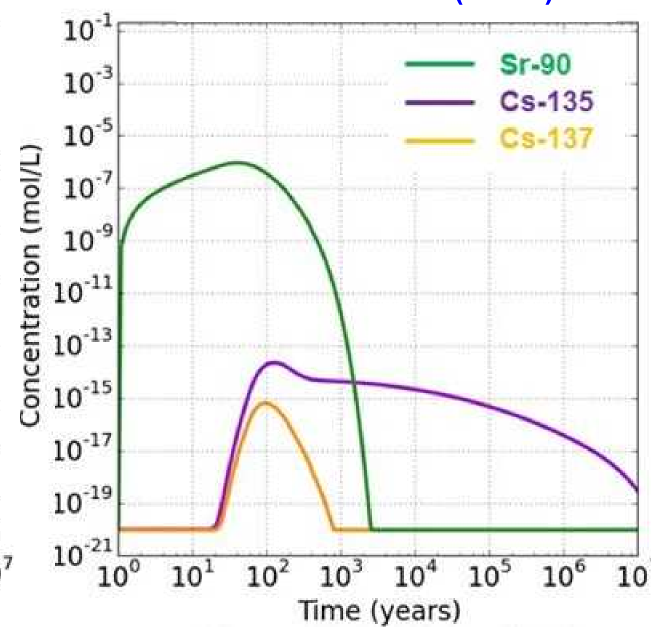
Nominal Scenario Deterministic Results – Dissolved Concentrations (mol/L) [PFLOTRAN]

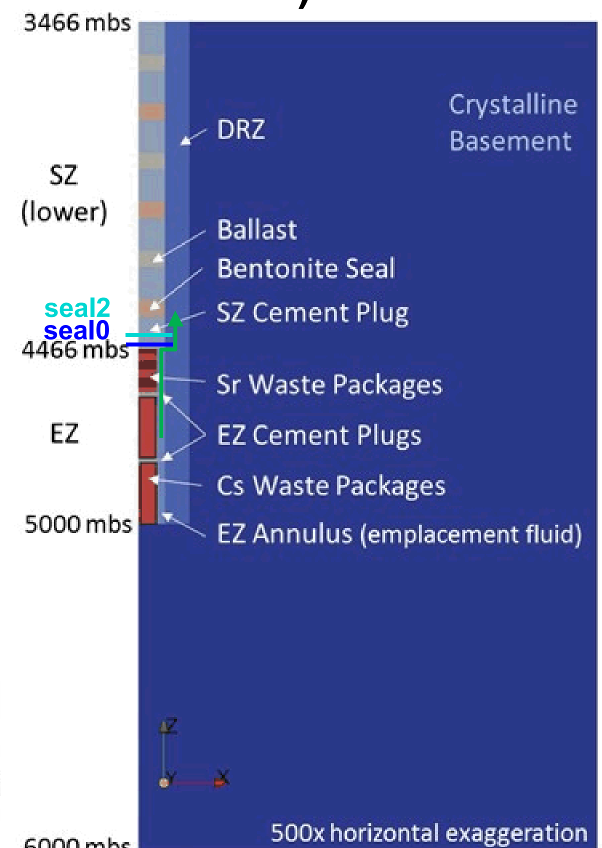
- **< ~100 yrs = Thermally-induced upward advection**
  - Highest in EZ annulus, overlying seal diverts flux to DRZ
- **> ~100 yrs = Slow diffusion**
- **Concentrations in SZ cement plug at 2 elevations (seal2 and seal0)**
  - Concentrations in DRZ at same elevations are similar

In SZ Cement Plug at z=4438.4 m (seal2)



In SZ Cement Plug at z=4463.4 m (seal0)

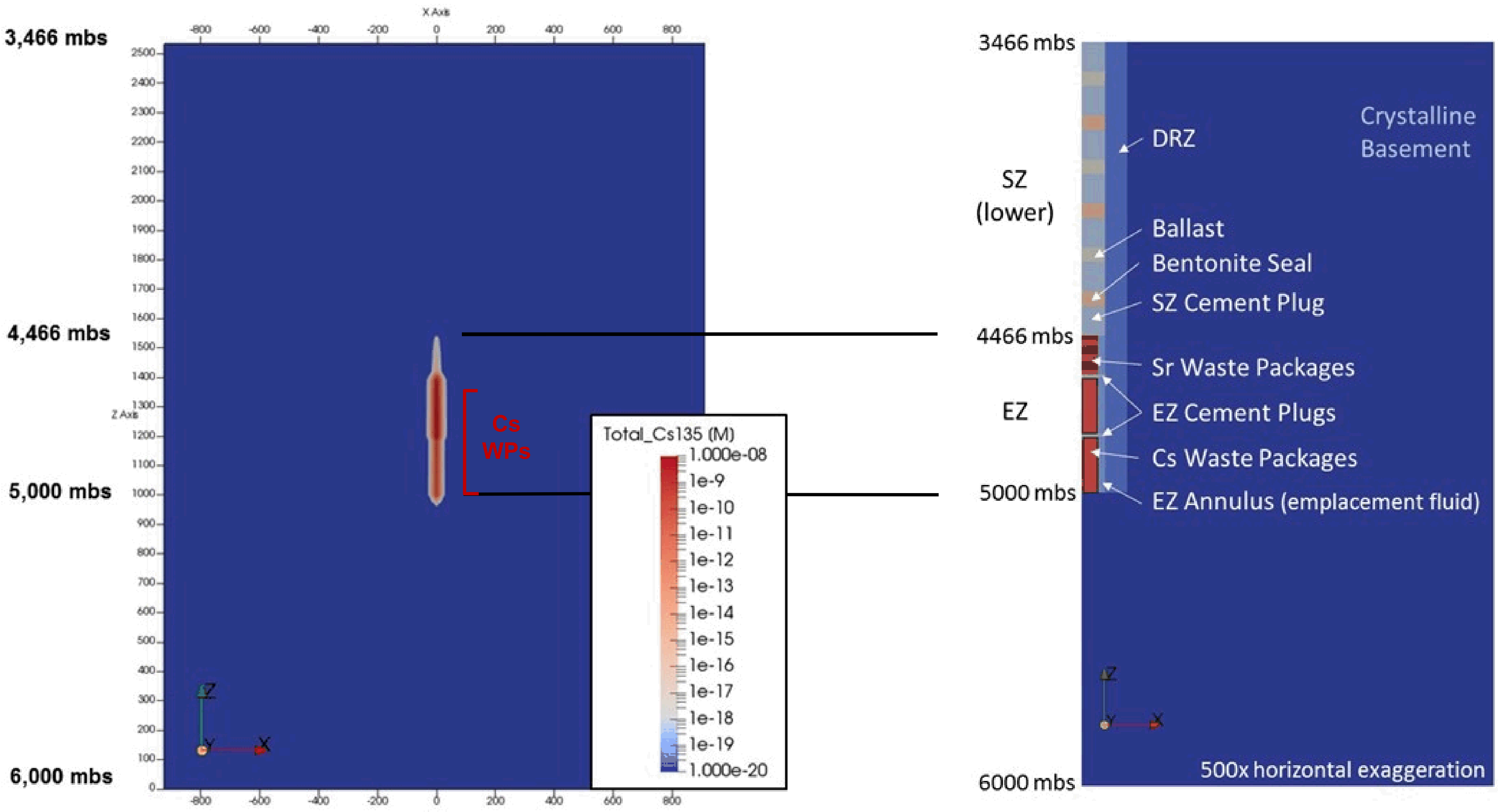




from Freeze et al. (2016), Figure 5-6

Nominal Scenario Deterministic Results – Dissolved Concentrations (mol/L) [PFLOTRAN]

- **Dissolved Concentration of ^{135}Cs at 10,000,000 years**
  - Minimal migration beyond Emplacement Zone



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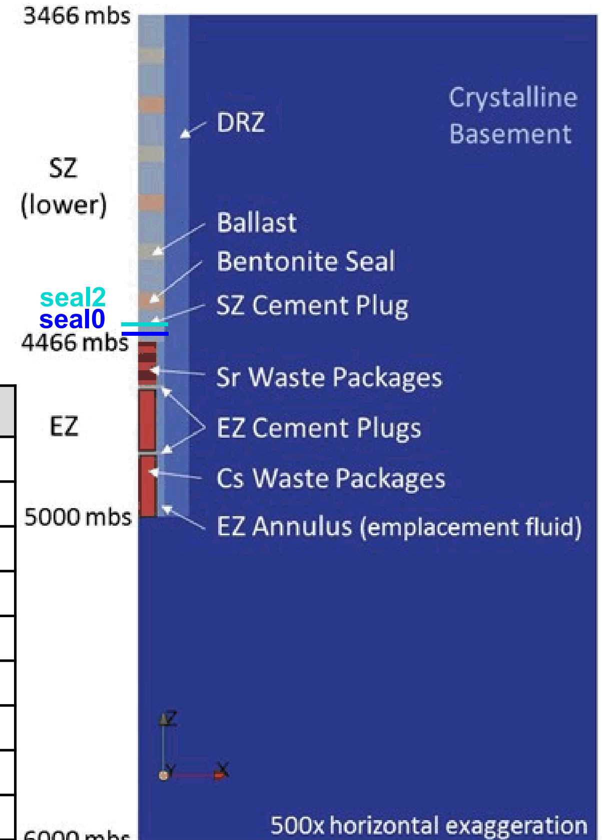
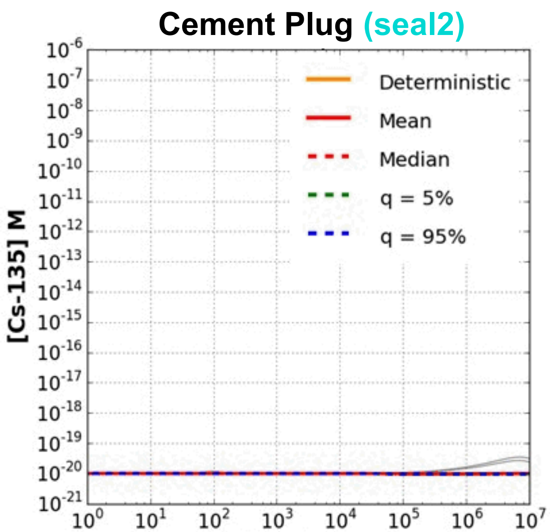
Nominal Scenario Probabilistic Results – [PFLOTRAN / DAKOTA]

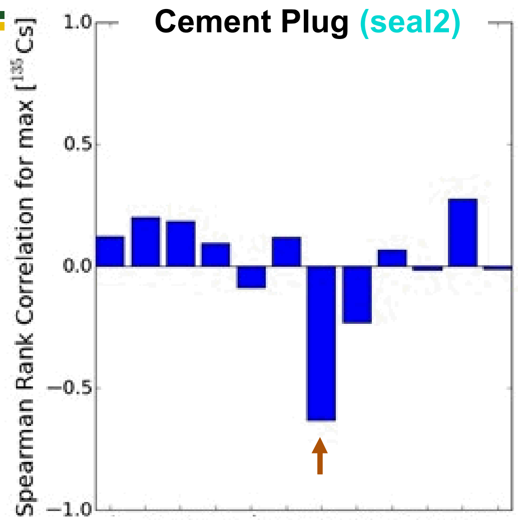
- **100 realizations with 12 sampled parameters**
- **Sensitivity (Spearman rank correlation) to maximum ^{135}Cs concentration**
  - calculated at several locations
  - shown at seal0 and seal2 in the cement plug

Parameter	ID	Range	Units	Distribution
Bentonite Permeability	kseal	10^{-20} – 10^{-16}	m^2	log uniform
Cement Permeability	kcement	10^{-20} – 10^{-16}	m^2	log uniform
DRZ Permeability	kdrz	10^{-18} – 10^{-15}	m^2	log uniform
WP Tortuosity	tWP	0.01 – 1.0	--	log uniform
Bentonite Porosity	pseal	0.40 – 0.50	--	uniform
Cement Porosity	pcement	0.15 – 0.20	--	uniform
DRZ Porosity	pdrz	0.005 – 0.01	--	uniform
WP Breach Time	breach	1 – 100	yr	uniform
Cs K_d Bentonite	KdCs_s	120 – 1000	ml/g	uniform
Sr K_d Bentonite	KdSr_s	50 – 3000	ml/g	uniform
Cs K_d Crystalline/DRZ	KdCs_g	5 – 40	ml/g	uniform
Sr K_d Crystalline/DRZ	KdSr_g	0.4 – 3	ml/g	uniform

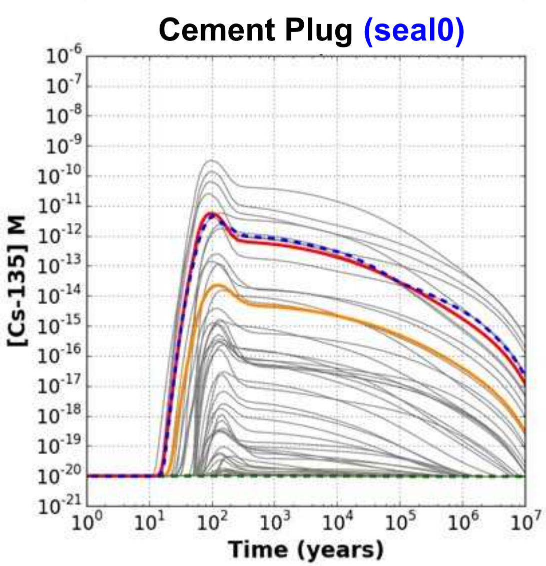


Nominal Scenario Probabilistic Results – [PFLOTRAN / DAKOTA]

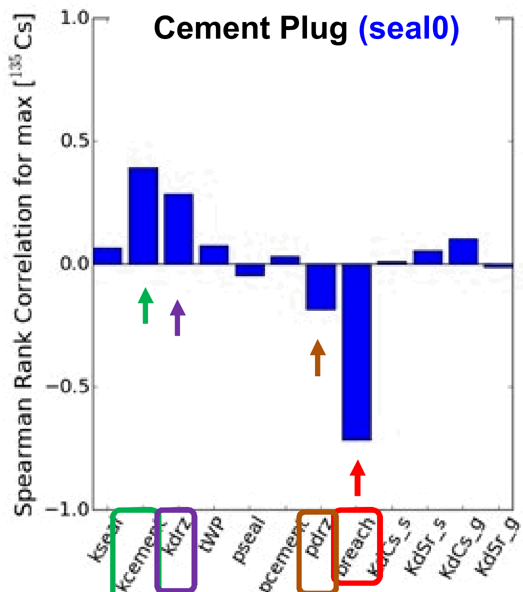




- **Key parameters for seal2**
  - Similar to seal0 but rank correlations not as “robust” due to minimal number of realizations with “non-zero” max. concentration



from Freeze et al. (2016), Figure 5-9



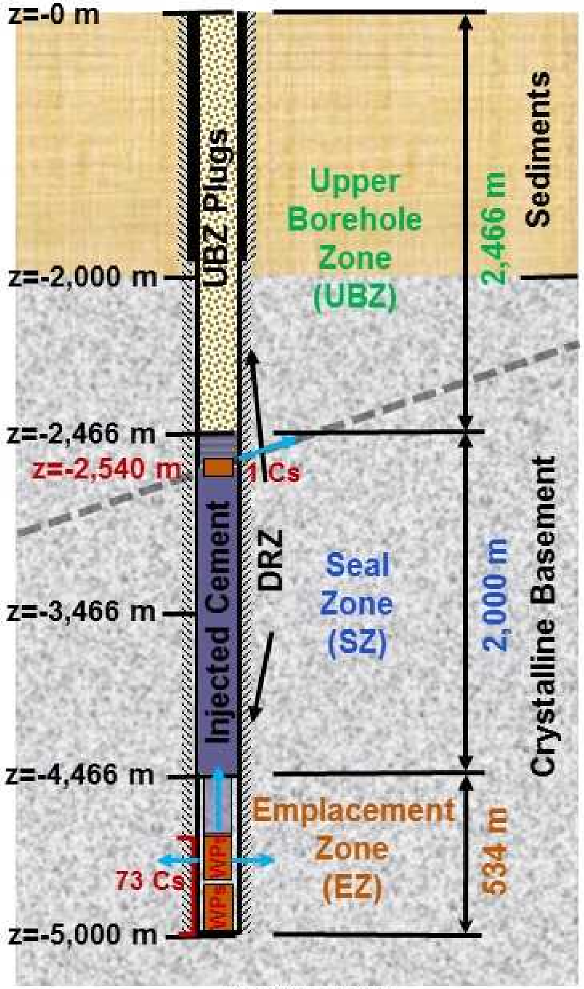
from Freeze et al. (2016), Figure 5-11

- **Key parameters for seal0**
  - WP breach time
  - Cement plug permeability
  - DRZ permeability
  - DRZ porosity

Post-Closure PA – Disturbed Scenario

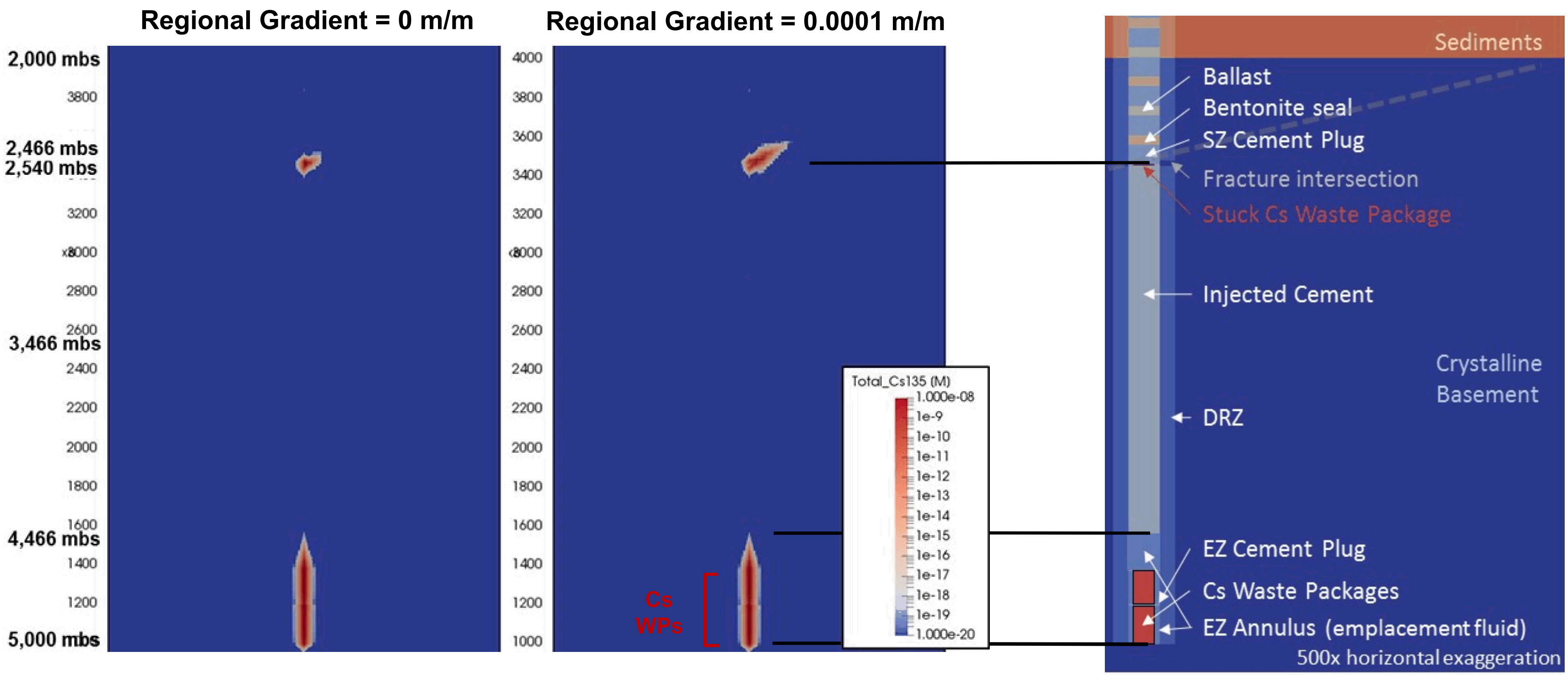
Post-Closure Release Pathways

- Undisturbed pathways from nominal scenario
- WP (74th Cs) stuck in borehole-intersecting fracture
  - fracture: $k = 10^{-14}$ m^2, $D_e = 1 \times 10^{-12}$ m^2/s
  - cement injected below stuck package
  - SZ and UBZ sealed above stuck package
- Regional flow gradient in crystalline basement
  - case 1 = 0 m/m (same as nominal scenario)
  - case 2 = 0.0001 m/m
- Other disturbed scenarios
  - Seismic, igneous, human intrusion



Disturbed Scenario Deterministic Results – Dissolved Concentrations (mol/L) [PFLOTRAN]

- **Dissolved Concentration of ^{135}Cs at 10,000,000 years**
  - Advection of ^{135}Cs up fracture (~200 m) due to regional gradient
  - ^{135}Cs still remains well below sedimentary overburden



Summary and Conclusions

- **Preliminary results from post-closure PA calculations suggest minimal radionuclide migration beyond the emplacement zone and zero dose at biosphere**
  - Radionuclide mobility is limited by:
    - Borehole seals that can maintain their physical integrity for the time period of thermally-induced upward advection (a few hundred years)
    - Slow diffusion after the thermal period
    - Geochemically reducing conditions that enhance sorption.
  - Engineered barrier performance (WP, WF, seals) is adequate for post-closure safety, but could be engineered to be more robust, as needed

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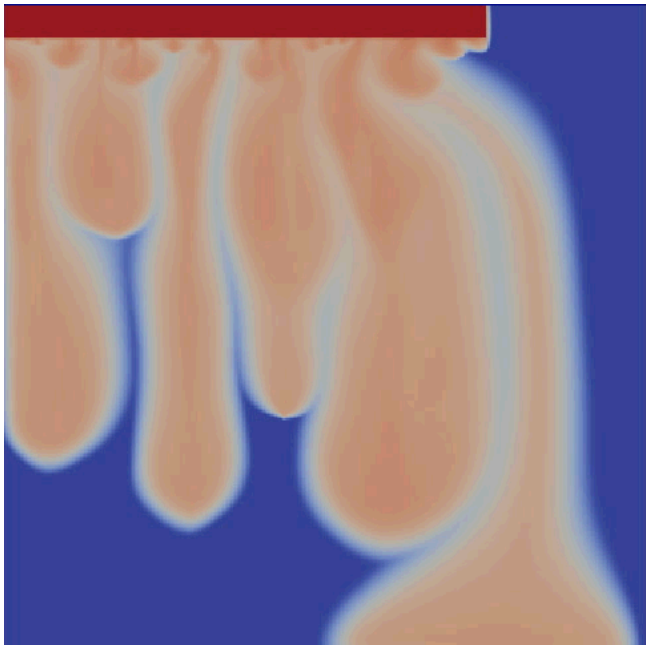
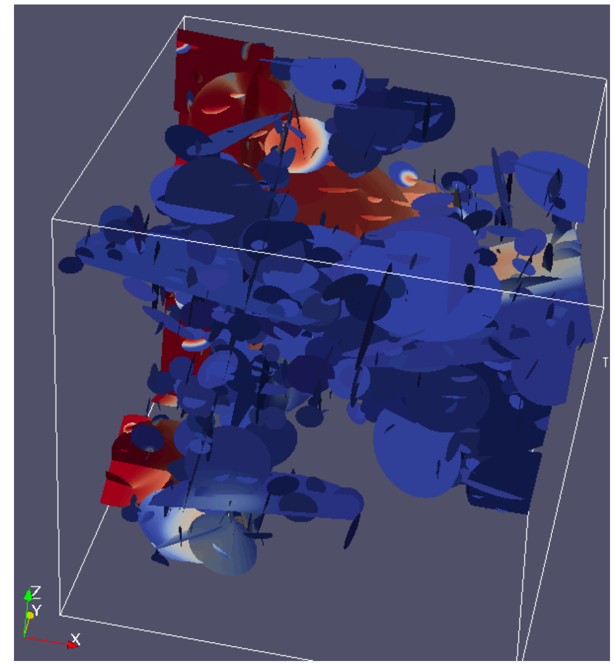
Next Steps

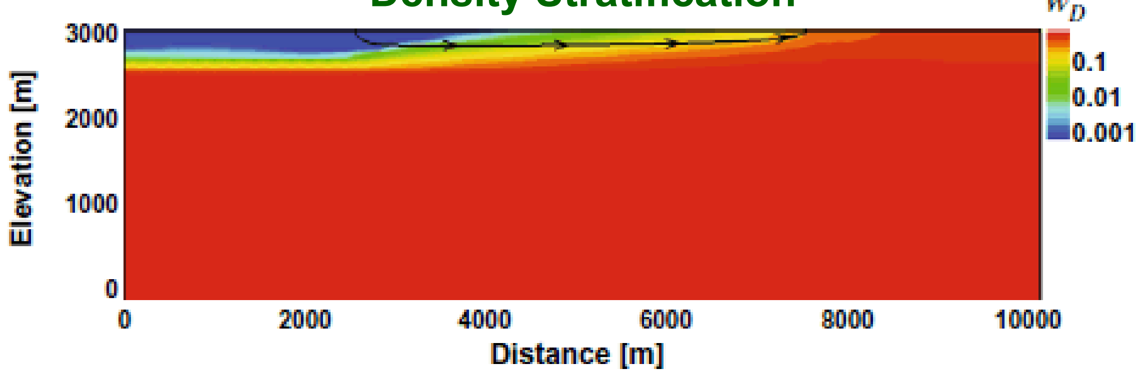
Salinity-Dependent Density



High Permeability Pathways



Regional Flow with Density Stratification



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