Probabilistic Performance Assessment for Deep Borehole Disposal of Cs/Sr Capsules – 17143

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ABSTRACT

The US Department of Energy (DOE) performed an assessment of disposal options for spent nuclear fuel (SNF) and high-level radioactive waste (HLW) that recommended the consideration of deep borehole disposal (DBD) of smaller DOE-managed waste forms, such as cesium (Cs) and strontium (Sr) capsules. To further assess the safety and viability of the DBD concept, post-closure performance assessment (PA) analyses were performed for DBD of Cs/Sr capsules.

The post-closure PA included a reference design concept for Cs/Sr capsule disposal, feature, event, and process (FEP) analysis, scenario development, and modeling using the PFLOTRAN code. PA simulations were run for both nominal and disturbed scenarios for long-term radionuclide transport away from the deep disposal borehole.

The nominal (expected) post-closure release scenario included FEPs for short-duration (a few hundred years) thermally-induced upward fluid flux through the borehole seals and/or disturbed rock zone (DRZ) followed by longer-term slow diffusive transport. Simulations included a baseline deterministic run and a set of probabilistic realizations (using Latin Hypercube Sampling (LHS) from parameter distributions) to examine the sensitivity and importance of the long-term radionuclide transport to processes and parameters such as: waste package durability; seal porosity and permeability, disturbed rock zone (DRZ) porosity and permeability; and radionuclide sorption in the seal materials, DRZ, and crystalline host rock.

The disturbed scenario included a waste package “stuck” in the crystalline basement above the emplacement zone near a hypothetical borehole-intersecting fracture. Simulations included two deterministic runs to examine the sensitivity to the regional head gradient.

The nominal and disturbed scenario PA results suggest that a favorable safety case can be developed for DBD of Cs/Sr capsules and helped to identify key areas of uncertainty, which in turn can inform future DBD research and development (R&D) activities, including a field demonstration project.

INTRODUCTION

DBD for the geologic isolation of SNF and/or HLW has been considered for many years, beginning with evaluations by the US National Academy of Sciences in 1957 [1]. Although efforts by the US and the international community over the last half-century have primarily focused on mined geological repositories, evaluations of DBD have periodically continued in several countries [2, Table 1-1].
From 2009 to 2012, an updated conceptual evaluation of DBD and a preliminary

performance assessment were completed [3], a reference design and operations methodology were developed using available drilling technology [4], and site characterization methods were analyzed [5]. These studies, which focused on DBD of commercial SNF, identified no fundamental flaws regarding safety or implementation of the DBD concept.

In 2013, DOE developed a strategy for management and disposal of SNF and HLW and performed an assessment of disposal options that recommended consideration of DBD of smaller DOE-managed waste forms, such as Cs and Sr capsules [6, 7]. In accordance with this recommendation, the DOE Office of Nuclear Energy (DOE-NE) is currently investigating the feasibility of DBD as one disposal alternative, along with R&D for mined repositories in salt, granite, and argillites, as part of the Used Fuel Disposition Campaign (UFDC). A DBD R&D roadmap was developed by the UFDC [8]; ongoing R&D activities [9, 10] include plans for a Deep Borehole Field Test (DBFT) [11, 12, 13, 14].

Deep Borehole Disposal Concept

The DBD concept, generalized in Fig. 1, consists of drilling a large-diameter borehole into crystalline basement rock to a depth of about 5,000 m, placing waste packages in the lower emplacement zone portion of the borehole, and sealing the upper portion of the borehole. As shown in Fig. 1, waste in a DBD system is several times deeper than typical mined repositories (e.g., Onkalo and WIPP) and is well below the typical maximum depth of fresh groundwater resources, indicated by the dashed blue line.

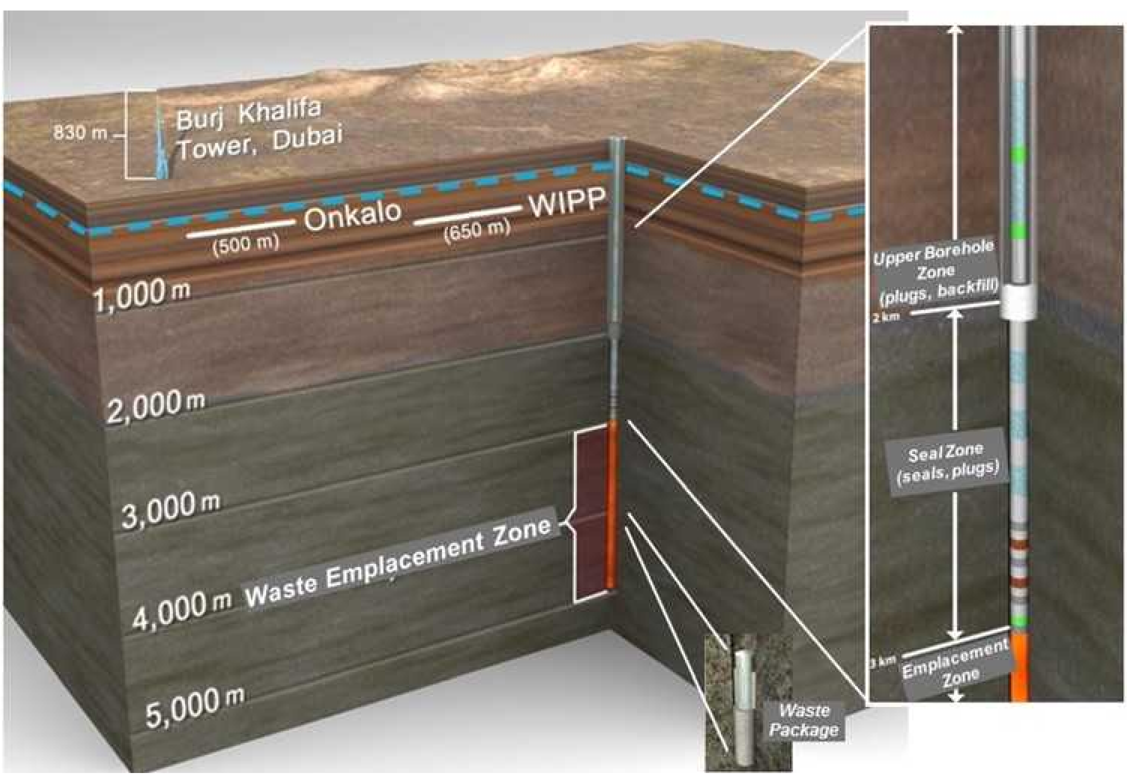


Fig. 1. Generalized schematic of the deep borehole disposal concept.

Safety of the DBD concept relies primarily on the natural barriers (great depth of burial and the isolation provided by the deep natural geological environment) and, to a lesser extent, on the engineered barriers (the durability of the waste packages and waste forms and the integrity of the borehole seals). In contrast, mined geological repositories, with the possible exception of those located in extensive salt or argillaceous formations, rely on engineered barriers such as waste packages and/or buffer material to a greater degree.

Several design alternatives exist that satisfy this basic concept, dependent on a variety of factors, most notably the size and characteristics of the waste form and packaging. DBD of SNF has been examined previously [3, 9, 16], this study focuses on DBD of Cs/Sr capsules.

DEEP BOREHOLE DISPOSAL REFERENCE CASE

Reference Design

The reference design concept for Cs/Sr capsule disposal (Fig. 2) includes a 5,000-m deep borehole with a bottom-hole (emplacement zone) diameter of 0.311 m (12.25 in) [2, 13]. This design is expected to be achievable in crystalline rocks with currently available commercial drilling technology.

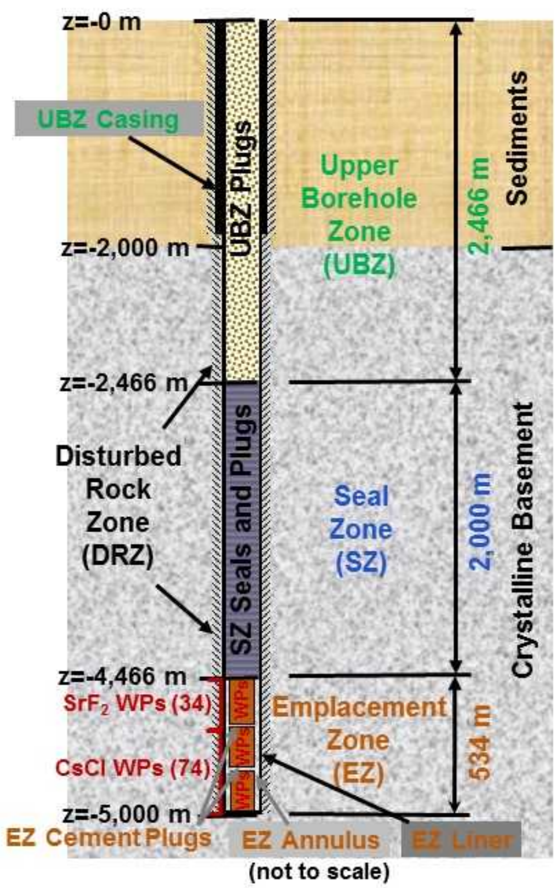


Fig. 2. Baseline deep borehole disposal concept for Cs/Sr capsules.

The DOE-managed inventory includes 1,335 Cs capsules and 601 Sr capsules currently stored at the Hanford Waste Encapsulation and Storage Facility that are all less than 0.09 m (3.5 in) in diameter [7]. These capsules contain short-lived Sr-90 and Cs-137, and long-lived Cs-135; other radionuclides have decayed away [15].

For the reference design [2, 13], waste packages containing the Cs/Sr capsules are placed in the lower, emplacement zone (EZ) portion of the borehole (between 4,466 m and 5,000 m depth). Each carbon steel waste package is assumed to contain 18 Cs or Sr capsules, stacked in 6 layers of 3 capsules (3-packs) each. Each waste package would have an outside diameter of 0.219 m (8.625 in) and a total length of 4.76 m, which includes 3.76 m for the 6 layers of capsules, a 0.3-m long fishing neck (to facilitate retrieval during operations), and a 0.7-m-long impact limiter (to minimize damage from drops). With this reference design (other configurations are possible), 108 waste packages would be required to accommodate all of the Cs/Sr capsules (74 for the Cs capsules and 34 for the Sr capsules), and all of the waste packages would fit in a single borehole with an EZ 0.311 m (12.25 in) in diameter and 534 m long (this length includes 10-m long cement plugs above the 40^{th} and 80^{th} waste packages for structural support).

A perforated steel liner is assumed to extend the length of the EZ. A temporary guidance casing from the surface will be designed to work in conjunction with the EZ liner to facilitate smooth emplacement of waste packages. The EZ also includes annular spaces between the stacked waste packages and the EZ liner and between the EZ liner and the borehole wall. For the reference design, the EZ annular regions are assumed to be filled with high density brine, similar to formation fluid.

The upper portion of the borehole includes a seal zone (SZ) entirely within the crystalline basement rock, where seals and plugs (bentonite seals, cement plugs, silica sand/crushed rock ballast) will be emplaced directly against borehole wall, and an upper borehole zone (UBZ) primarily within the sedimentary overburden, where plugs (cement alternating with ballast) will be emplaced against the cemented casing. For the reference design [2, 13], the SZ is a 2,000-m interval (between 2,466 m and 4,466 m depth). Seals in the SZ would act directly against the rock (the DRZ) to limit upward radionuclide transport; cement plugs in the SZ would minimize chemical interaction between adjacent seals.

Conceptual Model and Parameters

Key processes occurring in each of DBD system components were identified through FEP analysis [2, Section 5.2.1 and Appendix E]. The resulting nominal (i.e., undisturbed) scenario includes [2]:

- Thermal output and radioactivity from the Cs and Sr capsules assumes surface storage/aging until borehole emplacement in 2050.
- Waste forms (solid CsCl and SrF_2) that are assumed to degrade immediately after emplacement and do not perform any function (e.g., gradual dissolution) that would delay radionuclide release or transport. Unlimited solubility of Cs and Sr in groundwater is assumed.

- A 534 m EZ that contains 108 waste packages (74 for the Cs capsules and 34 for the Sr capsules). The cooler Cs waste packages are emplaced first, in the lower portion of the EZ. The waste packages are assumed to maintain structural integrity during surface handling and emplacement, but are assumed to degrade immediately after sealing and do not perform any function (e.g., gradual corrosion) that would delay radionuclide release or transport. For the deterministic simulation, this corresponds to a waste package breach time of one year after sealing. For the probabilistic simulations, waste package breach time is sampled between 1 year and 100 years.
- A 2,000 m SZ with permeability and porosity consistent with degraded properties of bentonite clay, cement plugs, and/or sand/crushed rock ballast. The overlying UBZ also has permeability and porosity consistent with degraded material properties.
- Sparsely fractured crystalline basement rock with low permeability and porosity and no regional flow gradient.
- A DRZ around the borehole that is assumed to have an elevated permeability with respect to the adjacent intact basement rock due to changes in stress induced by drilling.
- A temperature gradient with depth, calculated assuming a geothermal heat flux of 60 mW/m^2 at 6,000 m depth and an average annual surface temperature of 10°C. The resulting thermal gradient is ~25°C/km, with ambient temperatures of about 125°C at the top of the EZ and 140°C at the bottom of the EZ.
- The potential for advective and diffusive aqueous-phase transport. Radionuclide mobilization and transport properties are based on geochemically reducing conditions consistent with deep crystalline rock. (Consideration of gas-phase and/or colloidal transport is deferred to a future PA).

Material properties used to represent these DBD system features and processes in the nominal scenario simulations are summarized in Table I (parameter values for the baseline deterministic run) and Table II (parameter ranges for the probabilistic realizations).

The disturbed scenario derives from the nominal scenario with the following changes:

- A single Cs waste package is assumed to remain "stuck" in the crystalline basement above the EZ near a borehole-intersecting fracture. As a remedial measure, it is assumed that cement was injected (through the annulus outside the guidance casing) into the seal zone below the stuck package. Properties of the injected cement of listed in Table I.
- The properties of the borehole-intersecting fracture (Table I) are derived from a discrete fracture network (DFN) representation of a fracture system. The fracture was assumed to have a 30° dip, intersecting the borehole at a depth of 2,540 m (540 m below the base of sedimentary overburden). Two cases were analyzed: one with no regional head gradient (as in the undisturbed scenario), and one with a regional head gradient of 0.0001 m/m, driving flow up dip toward the sediments.

TABLE I. Material properties for deterministic simulations [2]

Material	Permeability (m^2)	Porosity (-)	Effective Diffusion Coeff.[a] (m^2/s)	Thermal Cond. (W/m·K)	Heat Capacity (J/kg·K)	Sr K_d [b] (L/kg)	Cs K_d [b] (L/kg)
Waste Package	1×10^{-16}	0.43	4.3×10^{-10}	17	500	0	0
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
Injected Cement[c]	1×10^{-16}	0.25	6.3×10^{-11}	1.7	900	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
Fracture[c]	1×10^{-14}	8×10^{-6}	1.0×10^{-12}	2.5	880	1.7	22.5
Sediments	1×10^{-15}	0.20	4.0×10^{-11}	2.0	800	50	120

[a] Effective diffusion coefficient = (free water diffusion coefficient) × (tortuosity) × (porosity)
[b] K_d = distribution coefficient (for linear sorption)
[c] Disturbed scenario only

TABLE II. Undisturbed scenario sampled parameters and ranges [2]

Parameter	Range	Units	Distribution
Bentonite Permeability	10^{-20} – 10^{-16}	m^2	log uniform
Cement Permeability	10^{-20} – 10^{-16}	m^2	log uniform
DRZ Permeability	10^{-18} – 10^{-15}	m^2	log uniform
WP Tortuosity	0.01 – 1.0	--	log uniform
Bentonite Porosity	0.40 – 0.50	--	uniform
Cement Porosity	0.15 – 0.20	--	uniform
DRZ Porosity	0.005 – 0.01	--	uniform
WP Breach Time	1 – 100	yr	uniform
Cs K_d bentonite	120 – 1000	L/kg	uniform
Sr K_d bentonite	50 – 3000	L/kg	uniform
Cs K_d crystalline	5 – 40	L/kg	uniform
Sr K_d crystalline	0.4 – 3	L/kg	uniform
Cs K_d DRZ	5 – 40	L/kg	uniform
Sr K_d DRZ	0.4 – 3	L/kg	uniform

POST-CLOSURE PERFORMANCE ASSESSMENT – NOMINAL SCENARIO

Baseline Deterministic Simulation

The PA model domain for the nominal scenario (Fig. 3) is two-dimensional (2-D) axisymmetric with a radius of approximately 1,000 m (923.627 m), and a height of 2,534.08 m. The base of the 534.08-m long EZ lies at 5,000 m below the land surface (mbs); the EZ contains 108 4.76-m long waste packages and 2 10-m long cement plugs. To minimize peak temperature in the EZ, the cooler Cs waste packages are emplaced in the lower portion of the EZ, where the ambient temperature is higher, overlain by the hotter Sr waste packages. The EZ liner is not modeled. Instead, the entire annular space between the waste packages and the borehole wall (DRZ) is modeled as a brine-filled EZ annulus.

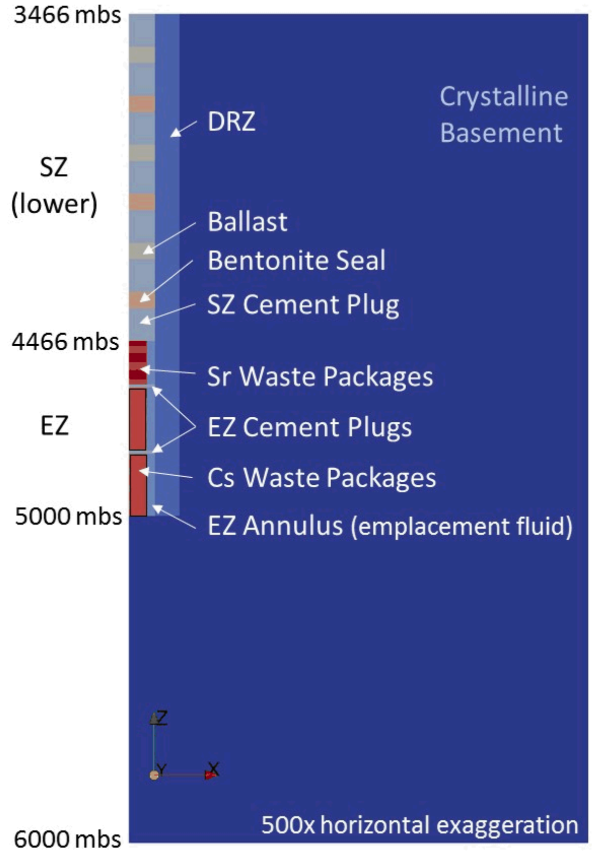


Fig. 3. A portion of the DBD PA model domain for the nominal scenario.

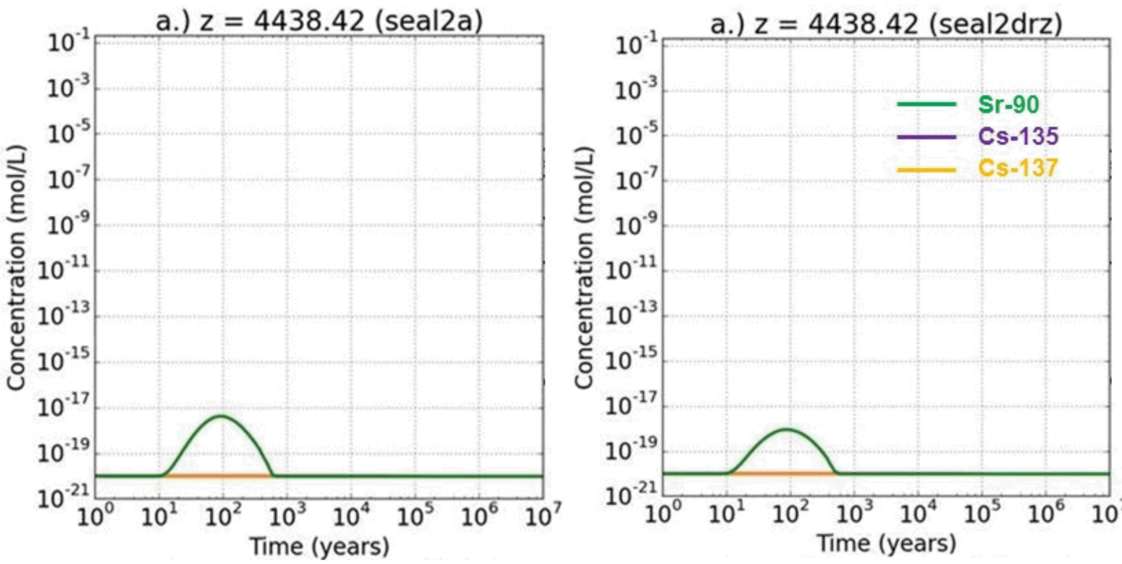
The PA model for the nominal scenario includes only the lower portion of the SZ, a 1,000-m interval consisting of alternating lengths of cement, bentonite, and ballast, extending from the top of the uppermost waste package in the EZ to the top of the model domain. Two 100-m-long cement plugs sit at the top and bottom of the lower seal zone; five additional cement plugs (each 100-m long) separate alternating 50-m lengths of bentonite seal and ballast material. A DRZ, 0.15 m in width, envelopes the entire length of the borehole.

Numerical simulations of thermal-hydrology and radionuclide mobilization and transport for the reference case were implemented with PFLOTRAN, an open source, massively parallel subsurface flow and reactive transport code [17], in a high-performance computing environment. The probabilistic simulations were run using DAKOTA, an analysis package for uncertainty quantification, sensitivity analysis, optimization, and calibration in a parallel computing environment [18]. At the time of waste package breach, the entire (decayed) inventory of Cs-137, Cs-135, and/or Sr-90 in a waste package is assumed to be present in solution within the waste package cell, based on the reference case assumption of unlimited solubility of Cs and Sr in the EZ. Instantaneous dissolution of the entire 18-capsule inventory (in 2050) in a waste package into the void space of the waste package results in a dissolved concentration (source term) of approximately 0.83 mol/L for Cs (from Cs-135 and Cs-137) and approximately 0.25 mol/L for Sr (from Sr-90). Unlimited solubility for Cs and Sr is also assumed in the PA model domain beyond the EZ.

Predicted temperatures, fluid fluxes (specific discharge), and radionuclide concentrations for 10,000,000 years were captured at several observation point depths within the model domain, including: seal0 (4,463 mbs), 2.5 m above the EZ in the lowermost SZ cement plug; and seal2 (4,438 mbs), approximately 25 m above the EZ in the lowermost SZ cement plug.

Temperatures in the EZ, driven by the heat of radioactive decay, peak at ~3 years, reaching 240°C near the midpoint of the EZ [2]. The increase in temperature creates a thermally-driven upward fluid flux that includes effects from fluid thermal expansion (early fluxes of very short duration) and buoyant convection (later fluxes due to buoyancy of the hot fluid, which generally peak at the same time as temperatures, and are relevant to possible radionuclide transport) [13]. The buoyancy-driven flux is largest in the fluid-filled EZ annulus of the borehole. However, ~25 m above the top of the EZ (at seal2 depth), buoyancy-driven vertical specific discharge does not exceed 0.0001 m/yr within the cement plug or 0.006 m/yr within the DRZ. The lack of significant buoyancy-driven fluid flux in the seal zone is apparent in the predicted radionuclide concentrations within the SZ. A very small concentration ($<10^{-17}$ mol/L) of Sr-90 travels approximately 25 m into the cement plug at the base of the SZ (Fig. 4a); the peak concentration of Sr-90 in the DRZ at the same elevation is even lower (Fig. 4b). The Cs waste packages are emplaced below the Sr waste packages. Due to the longer travel distance, neither the short-lived Cs-137 nor the long-lived Cs-135 travel as far as 25 m into the SZ through either the cement plug or the DRZ; both remain at the initial background concentration of 10^{-20} mol/L for the entire simulation duration.

Fig. 5 shows the Cs-135 concentrations throughout the model domain at 10,000,000 years. Most of the Cs-135 remains in the lower part of the EZ, where the 74 waste packages containing the Cs capsules were originally emplaced. The effects of the two 10-m long EZ cement plugs (centered at depths of ~4,805 mbs and ~4,604 mbs) on Cs-135 movement are also evident. Radionuclides diffuse laterally through the crystalline host rock away from the EZ. However, after 10,000,000 years, the Cs-135 concentration contour of 10^{-15} mol/L has only reached a radius of approximately 20 m beyond the EZ. No Cs-135 reaches the biosphere, so there is no dose.



(a) in the SZ cement plug **(b) in the DRZ**

Fig. 4. Radionuclide concentrations at seal2 depth (~25 m above the EZ) [2].

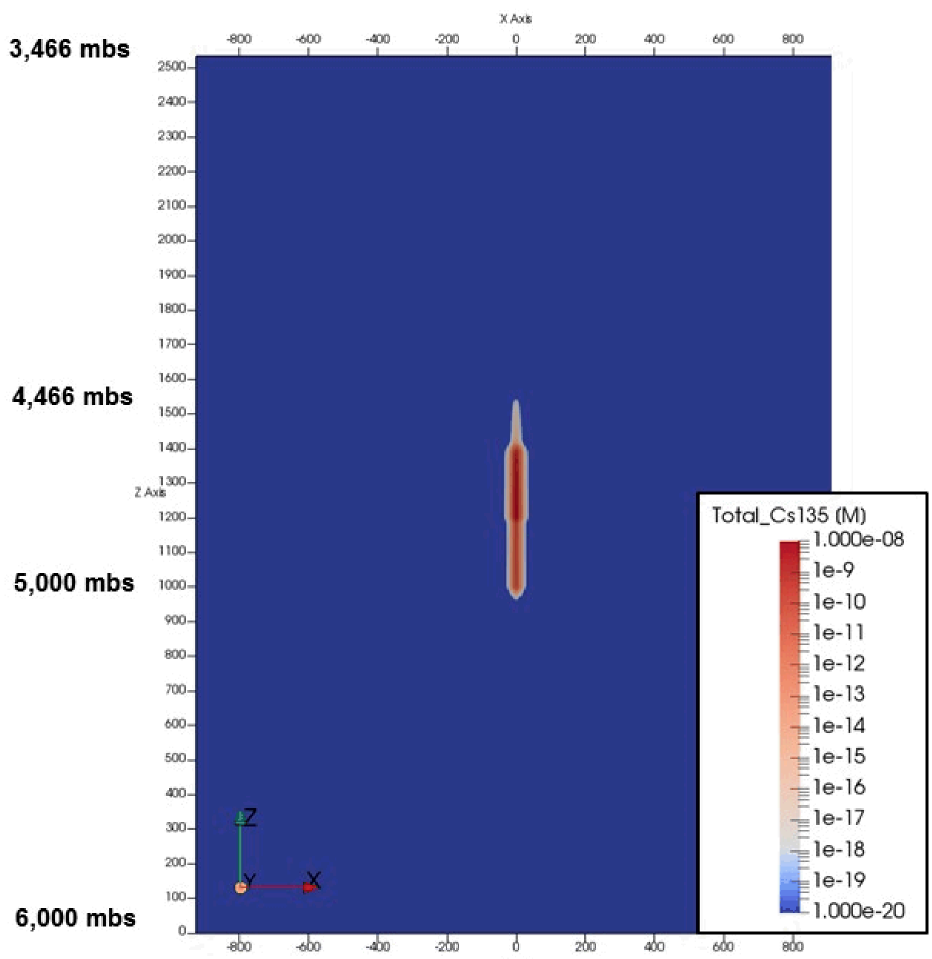


Fig. 5. Nominal scenario dissolved concentration of Cs-135 at 10,000,000 years [2].

Probabilistic Simulations

A suite of 100 probabilistic simulations were run to analyze uncertainty and sensitivity due to the parameters listed in Table II. The concentration of Cs-135 in the SZ cement plug at the seal0 depth (2.5 m above the EZ) was used as a performance metric. Horsetail plots show the uncertainty in predicted Cs-135 concentrations due to uncertainty in the sampled input parameters; concentration versus time is plotted for seal0 observation points in the SZ cement plug (Fig. 6). Concentrations do not exceed 10^{-9} mol/L in any realization at any time. Cs-135 concentrations in the cement plug at seal2 depth (~25 m above the EZ) do not exceed 10^{-19} mol/L in any of the realizations.

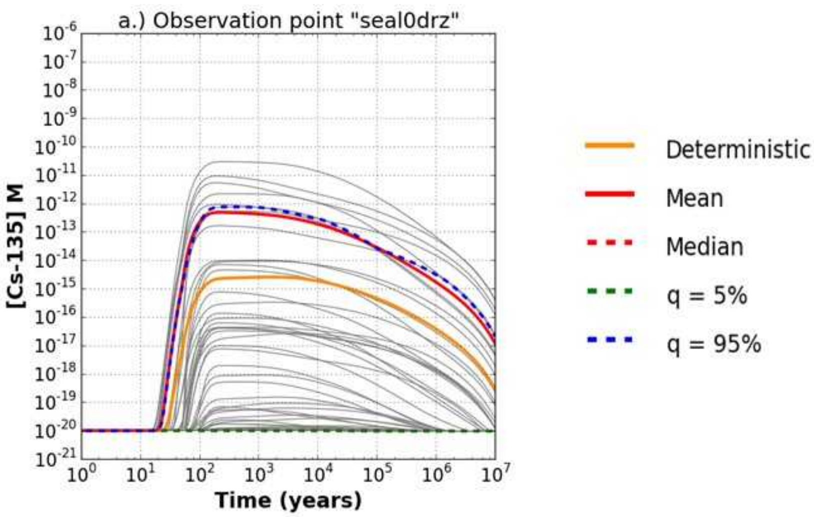


Fig. 6. Cs-135 concentration (mol/L) in the SZ cement plug at seal0 depth (2.5 m above the EZ) [2].

Sensitivity to sampled parameters was analyzed through the use of Spearman rank correlation coefficients relating the maximum Cs-135 concentration at the seal0 observation point to the sampled parameters (Fig. 7).

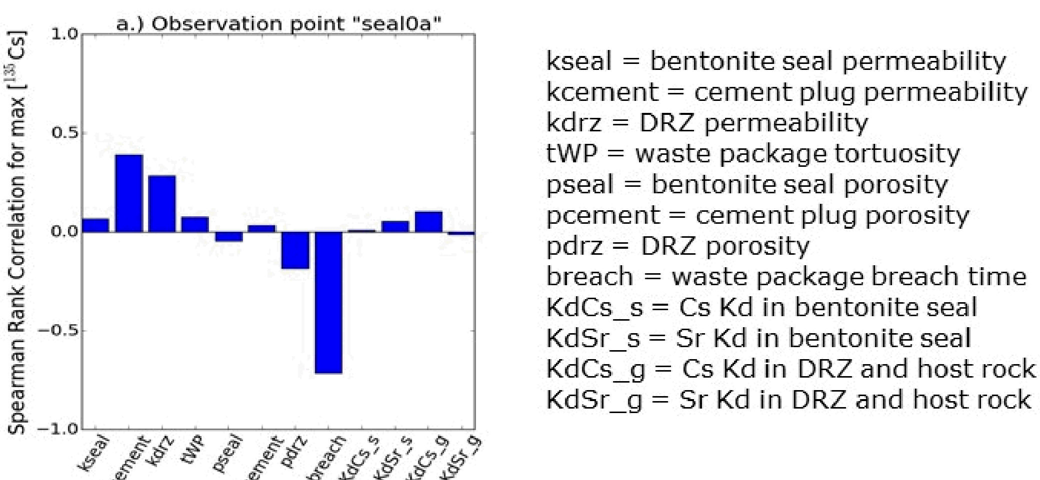


Fig. 7. Spearman Rank Correlation Coefficients relating maximum Cs-135 concentrations in the SZ Cement Plug to Sampled Parameters [2].

At this location in the cement plug, maximum Cs-135 concentration is most sensitive to waste package breach time. Delayed waste package breach results in lower predicted concentrations because the radionuclide releases from the waste packages occur after the early peak buoyancy-driven fluxes. The permeability of the cement plugs an of the DRZ plays a secondary role; the larger the permeability of these materials, the greater the maximum Cs-135 concentration.

POST-CLOSURE PERFORMANCE ASSESSMENT – DISTURBED SCENARIO

The disturbed scenario (Fig. 8) uses the same reference design, conceptual model, and parameters as the nominal scenario, except for the presence of (1) a hypothetical borehole-intersecting fracture in the crystalline basement above the EZ, (2) a single Cs waste package "stuck" near the borehole-intersecting fracture, and (3) cement injected below the stuck package instead of engineered seals and plugs.

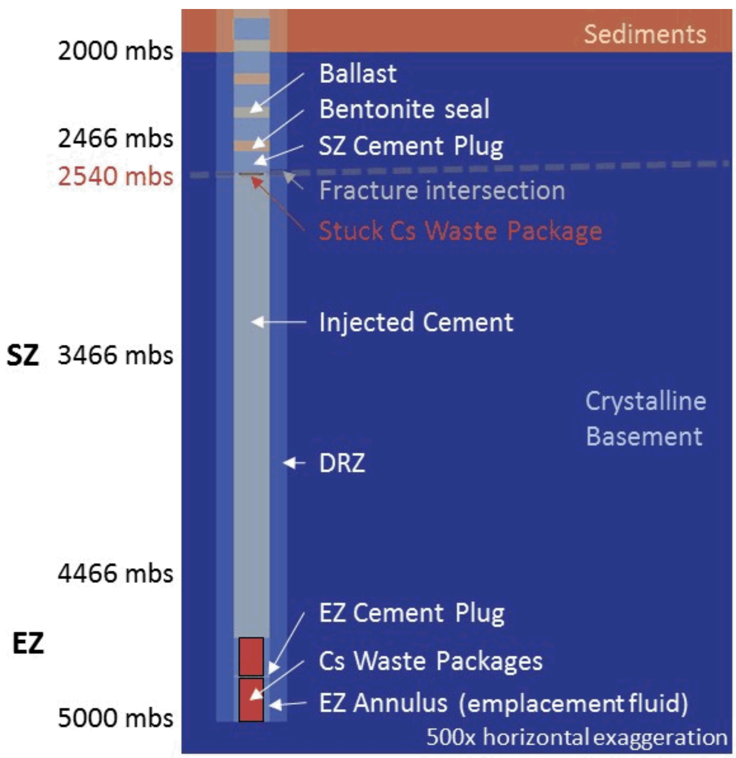
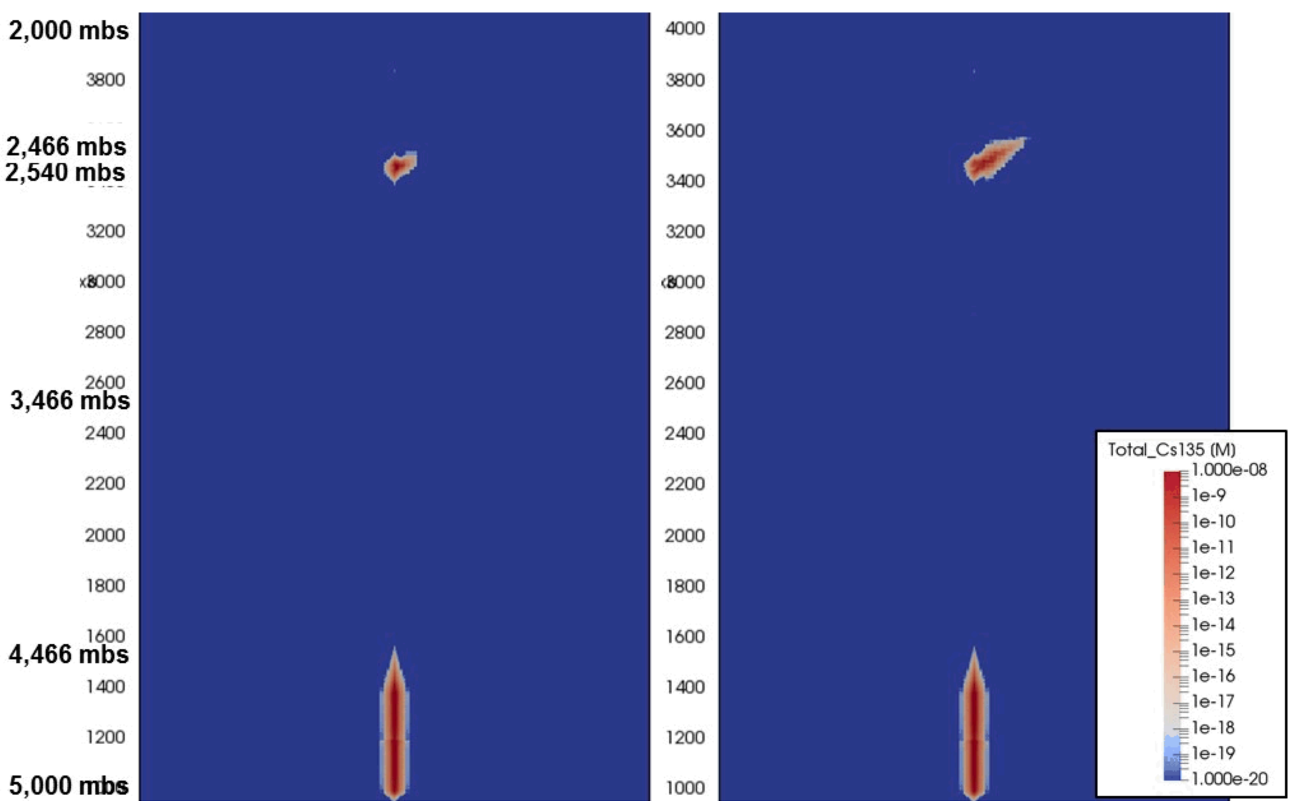


Fig. 8. A portion of the DBD PA model domain for the disturbed scenario.

The borehole-intersecting fracture was conceptualized as a 15-m thick brittle deformation zone with 30° dip that intersects the borehole at a depth of 2,540 m and has a transmissivity (1.5×10^{-6} m^2/s) at the upper end of values derived from packer tests in much shallower deformation zones (~500 m) in the well-characterized Forsmark metagranite [19]. Fracture properties (Table I) were conservatively chosen to create a transmissive feature at depth. However, it is likely that such a transmissive fracture intersecting the borehole would be identified during site characterization and/or drilling and would result in the borehole being abandoned or relocated.

For the disturbed scenario, the first 73 Cs waste packages are assumed to be emplaced in the lower portion of the EZ, and the final Cs waste package is assumed to get stuck in the guidance casing during emplacement at the depth of the fracture intersection (2,540 mbs). This location is within the upper SZ, 1,926 m above the top of the EZ and 540 m below the base of the sediments. It is assumed that (1) the stuck waste package cannot be fished, is left in place, and is breached, (2) the SZ seals and plugs below the stuck package are not present, the underlying SZ is instead filled with injected cement to the extent possible (with properties less robust than the engineered cement plugs), and (3) the SZ and UBZ above the stuck waste package are sealed and plugged as planned. Because of the stuck package, the 34 Sr waste packages are not present.

Deterministic simulations were run for two disturbed scenario cases: one with no regional head gradient, and one with a regional head gradient of 0.0001 m/m, driving flow up dip toward the base of the sediments. The presence of the fracture system necessitated the use of a 3D model domain for the undisturbed scenario runs. However, the 3D domain was conceptually equivalent to the 2D axisymmetric domain used in the nominal scenario simulations. Fig. 9 shows the Cs-135 concentrations throughout the model domain at 10,000,000 years for each of these cases.



(a) regional gradient = 0 m/m **(b) regional gradient = 0.0001 m/m**

Fig. 9. Disturbed scenario dissolved concentration of Cs-135 at 10,000,000 years.

As in the nominal scenario, most of the Cs-135 from the first 73 Cs waste packages remains in the lower part of the EZ. For the case with no regional head gradient (Fig. 9a), a small amount of Cs-135 is present in the fracture, due to early-time buoyant convection followed by slow diffusive transport from the single stuck waste package. For the case with a regional head gradient of 0.0001 m/m (Fig. 9b), Cs-135 is advected a distance of approximately 200 m up the fracture over the course of the 10-million-year simulation, but is still approximately 400 m below the sediments.

SUMMARY AND CONCLUSIONS

These preliminary nominal and disturbed scenario results suggest that there is minimal radionuclide migration and zero dose from deep borehole disposal of Cs/Sr capsules, even without any performance credit from the waste forms or waste packages. Key results include:

- Waste emplacement is deep; between 4,466 and 5,000 m depth in low-permeability crystalline basement rock with limited interaction with shallower groundwater.
- Radionuclide mobility is limited due to geochemically reducing conditions in the deep subsurface that enhances solubility and sorption.
- For the nominal (undisturbed) scenario, borehole seals can be engineered to maintain their physical integrity as permeability barriers, at least for a few hundred years, which is the time period of thermally-induced upward groundwater flow from decay heat. Long-term radionuclide movement is limited to slow diffusive transport.
- For the disturbed scenario, long-term advection of radionuclides away from a stuck waste package through a hypothetical borehole-intersecting transmissive fracture, driven by a regional head gradient in the crystalline basement, is still minimal.

These results, which will be further assessed as part of the Deep Borehole Field Test, suggest that a favorable safety case can be developed for deep borehole disposal of Cs/Sr capsules.

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