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# Generic Post-Closure Safety Assessment for Deep Borehole Disposal of Heat-Generating Waste – 20451

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## ABSTRACT

The deep borehole disposal (DBD) concept for high-activity waste 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 portion of the borehole – the waste emplacement zone – and sealing and plugging the upper portion of the borehole with a combination of bentonite, cement plugs, and sand or crushed rock ballast. The waste emplacement zone is several times deeper than typical mined repositories and is well below the typical maximum depth of fresh groundwater resources. Recent work describes a generic reference case for deep borehole disposal of Cs and Sr capsules stored at the Hanford Site. Two scenarios are described: an undisturbed (nominal) scenario, and disturbed scenario, in which a waste package is stuck adjacent to a transmissive fracture zone in crystalline basement. Simulations of the processes affecting radionuclide release and transport in the two scenarios provide the basis for quantitative post-closure performance assessment (PA) of the reference case. This paper presents a probabilistic PA of the stuck waste package scenario, i.e. uncertainties affecting radionuclide mobilization and transport are propagated through 200 realizations of a predictive model to quantify uncertainties in predicted radionuclide concentrations within the borehole and the fracture zone. Simulations predict no radionuclide transport in the borehole to distances greater than 100 m above the stuck waste package. An assumed lateral pressure gradient results in predictions of limited radionuclide transport in the fracture zone at a lateral distance of 200 m from the stuck waste package. These results complement previous results for the nominal scenario and contribute to the development of a generic safety case for DBD.

## INTRODUCTION

The deep borehole disposal (DBD) concept for high-activity waste 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 portion of the borehole – the waste emplacement zone – and sealing and plugging the upper portion of the borehole with a combination of bentonite, cement plugs, and sand or crushed rock ballast. The waste emplacement zone is several times deeper than typical mined repositories and is well below the typical maximum depth of fresh groundwater resources [1, 2]. Post-closure safety of the concept relies primarily on the natural barriers (depth of burial, isolation and residence time of deep groundwaters, low permeability of crystalline basement, etc.) and to a lesser extent on the integrity of engineered barriers including waste packages and borehole seals.

Freeze et al. [1, 2, 3, 4] developed a generic reference case for deep borehole disposal of the capsules containing CsCl and $SrF_2$ stored at the Hanford Site. The generic reference case specifies features of the engineered and natural barrier systems including: borehole and casing; waste inventory, waste form, and waste package; engineered components of the emplacement zone, seal zone, and upper borehole zone; crystalline basement host rock; and overlying sedimentary strata. Two scenarios are described: an undisturbed (nominal) scenario, and disturbed scenario, in which a waste package is stuck adjacent to a transmissive fracture zone in the crystalline host rock. Simulations of the processes affecting radionuclide release and transport in the two scenarios provide the basis for quantitative post-closure performance assessment (PA) of the reference case and contribute to the development of a generic safety case for DBD.

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The role of a performance assessment is to (i) quantify the performance of the disposal system, and (ii) take into account identified uncertainties to evaluate the level of confidence in the estimated performance [2]. The PA developed by Freeze et al. [1, 2, 3] includes propagation of uncertainties in properties and behavior of the DBD system in the undisturbed scenario, but considers only uncertainty in the driving force for regional flow in simulations of the disturbed scenario. In this paper, we extend the PA to include analysis of multiple uncertainties in properties and behavior of the DBD system in the disturbed scenario.

## REFERENCE CASE

The generic DBD concept is schematically illustrated in Figure 1. A 2-km thick sedimentary sequence overlies low-permeability crystalline basement. The borehole, which is drilled to a depth of 5 km, has a diameter of approximately 0.3 m in the waste emplacement zone. A disturbed rock zone (DRZ) extending the length of the borehole is expected to be more permeable than the intact host rock.

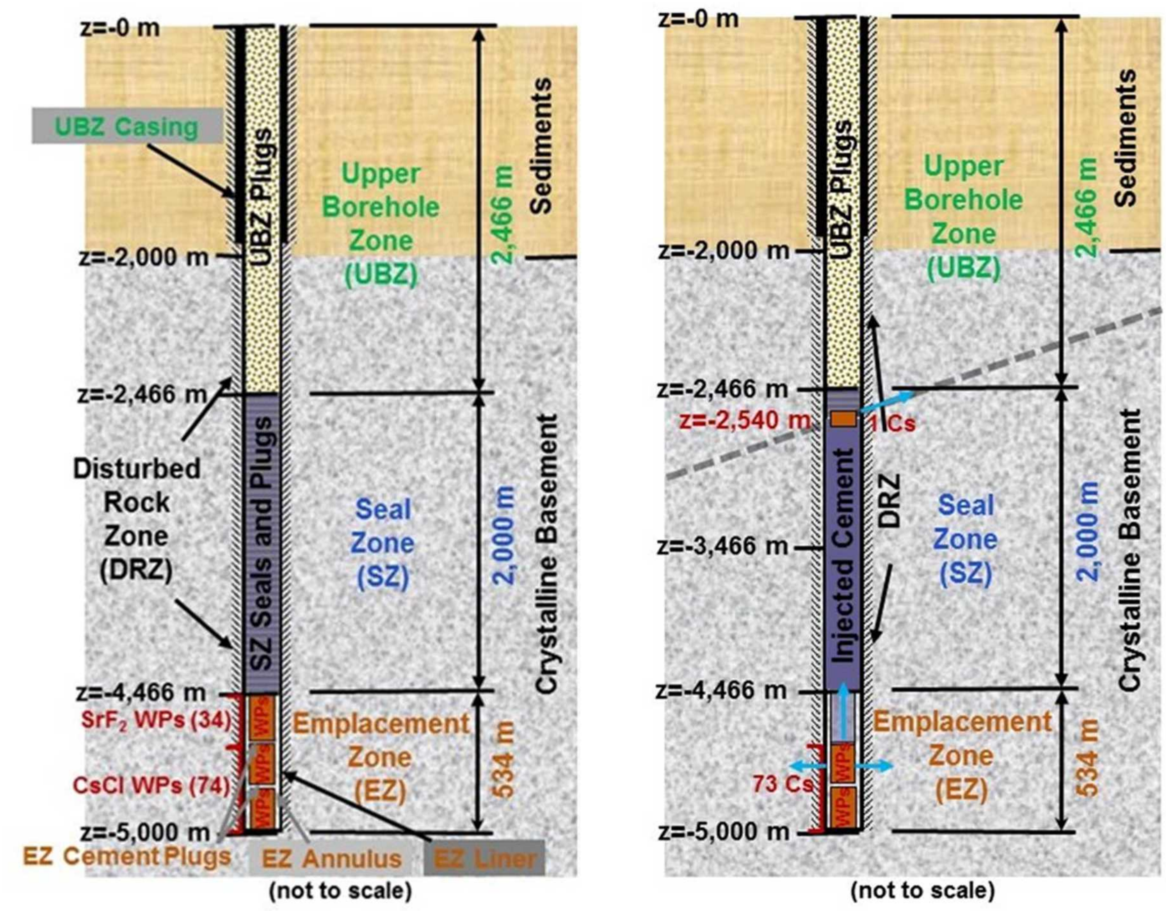


Figure 1. DBD schematics [2]: undisturbed scenario (left), and disturbed scenario (right).

In the undisturbed scenario, the 534-m long emplacement zone (EZ) contains 74 Cs waste packages and 34 Sr waste packages, the fluid-filled borehole annulus, a perforated steel casing, and two cement plugs emplaced to prevent waste packages at the base of the EZ being crushed by the weight of overlying waste packages. The seal zone (SZ) is a 2000-m interval above the EZ containing multiple bentonite seals bracketed by cement plugs and separated by zones of silica sand or crushed rock ballast. Guidance casing placed in the SZ to facilitate waste emplacement will be cut and removed prior to borehole sealing so that the seal materials lie in direct contact with the DRZ. Above the SZ, the upper borehole zone (UBZ) will be plugged with cement and ballast to inhibit fluid flow in the borehole and contribute to the stability of engineered components in the SZ.

In the stuck-waste-package scenario, 73 Cs waste packages are emplaced, and the 74$^{th}$ (last) Cs waste package is stuck near the top of the nominal SZ adjacent to a high-permeability fracture zone intersecting the borehole. Cement is injected into the SZ below the stuck waste package, and the SZ sequence of cement plugs, bentonite seals, and ballast is emplaced above the stuck waste package. In this scenario, no Sr waste packages are emplaced in the borehole. The remainder of this section describes the features of the disturbed scenario.

**Inventory, Waste Form, and Waste Package**

The radionuclide inventory in the stuck-waste-package scenario is the $^{135}$Cs ($t_{1/2} = 2.30\times10^{6}$ y) and $^{137}$Cs ($t_{1/2} = 30.0$ y) contained in the 1335 Cs capsules stored at the Hanford Site. Capsules vary in radioactivity and heat output. On average, a Cs capsule will contain 130 g $^{137}$Cs, 245 g $^{135}$Cs, and produce 54 W per capsule in 2050, the assumed year of waste emplacement [1].

The waste form is CsCl contained in double-walled capsules manufactured from either 316L stainless steel or corrosion-resistant Hastelloy C-276. Capsules are approximately 0.5 m in length and 0.07 to 0.08 m in diameter. The solubility of CsCl in brine is on the order of 10 mol/kg [1]. Reference case simulations conservatively assume instantaneous dissolution of CsCl upon waste package breach and unlimited solubility of Cs.

Each waste package holds 18 capsules, stacked in 6 layers of 3 capsules each. The waste package will be fitted with an impact limiter and a fishing neck, and have a total length of 4.76 m. The cylindrical part of the waste package is to be constructed of oilfield casing; the reference design assumes carbon steel casing with an outside diameter of 0.22 m and a wall thickness of 5 cm. The waste package will be designed to withstand hydrostatic pressure during emplacement, but may corrode through within tens of years [1].

**Emplacement Zone**

The EZ contains 73 waste packages, a 10-m-long cement plug emplaced above the 40$^{th}$ waste package, and a perforated steel liner (which is not simulated). The void spaces between stacked waste packages and the annular spaces between the waste packages, the EZ liner, and the borehole wall are assumed to be filled with a high-density brine of composition similar to that of formation fluid at depth. The density of the fluid in the EZ will change in response to chemical and thermal processes. Dissolution of the salt waste form will tend to increase fluid density; the increase in temperature due to the thermal output of the waste packages will tend to decrease fluid density. Simulations account for the influence of temperature on density, but do not account for the influence of dissolved solids. Radionuclide transport processes include advection and diffusion. Although cement and steel corrosion products may provide radionuclide sorption sites, sorption is conservatively neglected in the EZ.

**Seal Zone**

In the stuck-waste-package scenario, cement is injected between the guidance casing and the borehole wall to fill the nominal SZ below the stuck waste package. The length of the injected cement is 1900 m. Above the stuck waste package, a sequence of 3 50-m long bentonite seals alternating with 3 50-m long intervals of ballast is emplaced. Each interval of bentonite or ballast is supported by a 100-m long cement plug. The seal sequence is equal in length to the SZ in the undisturbed case, but is emplaced higher in the borehole.

Bentonite is a naturally-occurring montmorillonite clay of low permeability and high sorption capacity. It would be emplaced in the seal zone as dry compressed pellets or plugs, which would swell to fill the borehole as they hydrated. A successfully emplaced bentonite seal would have sufficient swelling pressure to form a tight seal with the borehole wall and to penetrate cracks in the DRZ, forming a barrier to radionuclide transport. As simulated, bentonite is the only material within the SZ with a non-zero $K_d$.

**Upper Borehole Zone**
The reference design calls for alternating intervals of cement plugs and ballast [1]. Numerical simulations assume the material properties of ballast between the uppermost cement plug of the SZ and the top of the model domain.

**Host Rock**
The basement host rock is assumed to be a sparsely fractured crystalline rock with a low porosity and permeability matrix, whose bulk hydraulic properties depend on fracture distribution and connectivity. Following Freeze et al. [1], a bulk permeability of $10^{-18}$ m$^2$, a porosity of 0.005, and an effective diffusion coefficient of $10^{-12}$ m$^2$/s are assumed. A disturbed rock zone with a radial thickness equal to one to two times the radius of the borehole is expected to have elevated permeability with respect to the permeability of the host rock matrix due to changes in stress induced by drilling. In the stuck waste package scenario, a high-permeability fracture zone with nominal thickness of 15 m and 30° dip intersects the borehole at a depth of 2,540 m.

Overlying sediments are simulated as a 2-km thickness of undifferentiated sediments. This simplified representation of a stratified sediment column is warranted, because the extent of radionuclide transport in all simulations is limited to crystalline basement.

## SIMULATION AND PROPAGATION OF UNCERTAINTIES
Simulations and analysis are performed with *Geologic Disposal Safety Assessment* (*GDSA*) *Framework*, an open-source software toolkit for probabilistic performance assessment of deep geologic disposal systems [5]. *GDSA Framework* is built on PFLOTRAN, a massively parallel multiphase flow and reactive transport simulator [6], and Dakota, an analysis package offering a wide variety of methods for optimization, uncertainty quantification, and sensitivity analysis in a high-performance computing environment [7]. Dakota's Latin hypercube sampling capability is used to generate 200 realizations of uncertain inputs to propagate through predictive simulations of coupled heat and fluid flow, advective and diffusive transport, sorption, and radioactive decay. Simulations run beyond any likely regulatory time period to $10^7$ years.

**Model Domain**
The three-dimensional, half-symmetry model domain (Figure 2) is 2,000 m in length ($x$), 1,000 m in width ($y$), and 6,000 m in height ($z$). The borehole is centered in $x$ and extends from the top of the model domain to 5000 m below the surface. A high-permeability fracture zone with nominal thickness of 15 m and 30° dip intersects the borehole at a depth of 2,540 m. Mapping the planar fracture zone into 15-m grid cells that are orthogonal in $x$ and $z$ results in a stair-stepped feature with a vertical extent of 30 m locally, as is the case immediately east of the borehole (Figure 2b). Fracture zone properties are applied where the fracture zone and DRZ intersect, thus the fracture zone (rather than the DRZ) provides a high-permeability vertical pathway extending 25 m above the stuck waste package on the east side of the borehole.

Initial temperature and pressure gradients are calculated assuming a geothermal heat flux of 60 mW/m$^2$, an average annual surface temperature of 10° C, and a lateral head gradient of -0.0001 m/m that drives flow from left (west) to right (east). Initial pressures and temperatures are held at all faces of the model domain, except the south face, at which no-flow (reflection) boundary conditions are applied. The initial concentration of $^{137}Cs$ and $^{135}Cs$ throughout the model domain is $10^{-20}$ mol/L. At inflow faces, this concentration is held constant; at outflow faces, a zero-gradient boundary condition is applied.

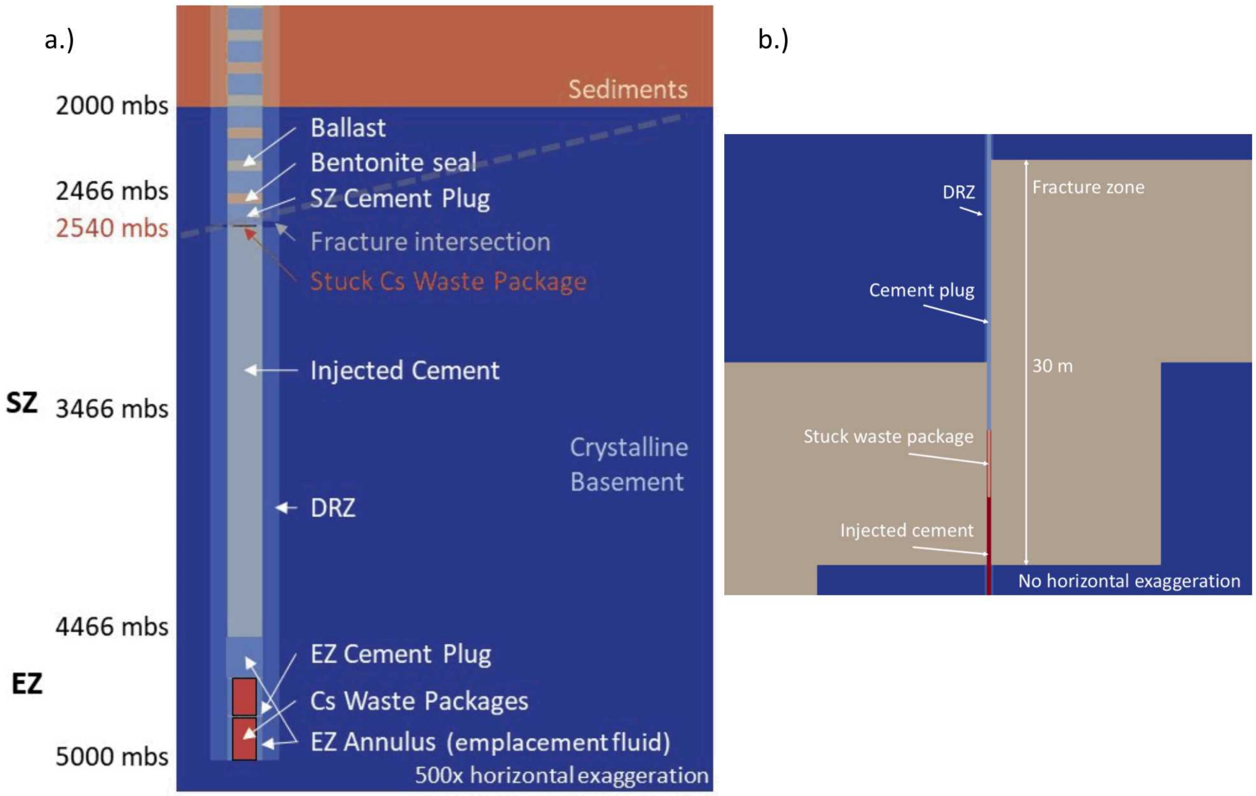


Figure 2. a.) Partial slice of the model domain for disturbed scenario [2]; b.) Close-up of the borehole/fracture intersection showing the relationship of the fracture zone to the stuck waste package and DRZ.

**Waste Package Heat and Radionuclide Source Terms**

A transient heat source term is associated with each waste package volume. The initial heat output of a Cs waste package is 978 W. The energy (watts per waste package) entering the model domain is updated periodically according to values in a lookup table. Between times specified in the lookup table, the energy source term is linearly interpolated.

Waste package breach time is sampled from a uniform distribution between 1 and 100 years. At the time of waste package breach, the entire (decayed) inventory of $^{137}Cs$ and $^{135}Cs$ is assumed to be present in solution within the waste package volume. Instantaneous dissolution of the 18-capsule inventory of $^{137}Cs$ and $^{135}Cs$ (in 2050) into the void space of a waste package would result in a dissolved Cs concentration of approximately 0.83 mol/L, well below the solubility limit.

**Material Properties**

The thermal properties of all materials and the hydraulic properties of the crystalline host rock, waste packages, brine-filled annulus, and ballast material are treated as constants [2, 3]. Porosity ($\phi$), permeability ($k$), and linear sorption coefficients ($K_d$) of selected materials are treated as uncertain variables (Table I).

TABLE I. Sampled variable distributions for propagation of uncertainty

| Variable | Description | Min | Max | Units | Distribution |
|---|---|---|---|---|---|
| kSeal | Bentonite $k$ | $10^{-20}$ | $10^{-16}$ | $m^2$ | log uniform |
| kPlug | Cement plug $k$ | $10^{-20}$ | $10^{-16}$ | $m^2$ | log uniform |
| kInj | Injected cement $k$ | $10^{-16}$ | $10^{-14}$ | $m^2$ | log uniform |
| kDRZ | DRZ $k$ | $10^{-18}$ | $10^{-15}$ | $m^2$ | log uniform |
| kFrac | Fracture zone $k$ | $10^{-17}$ | $10^{-14}$ | $m^2$ | log uniform |
| pSeal | Bentonite $\phi$ | 0.40 | 0.50 | – | uniform |
| pPlug | Cement plug $\phi$ | 0.15 | 0.20 | – | uniform |
| pDRZ | DRZ $\phi$ | 0.005 | 0.01 | – | uniform |
| bTime | Breach time | 1 | 100 | y | uniform |
| KdSeal | Cs $K_d$ in bentonite | 120 | 1000 | L/kg | uniform |
| KdGran | Cs $K_d$ in granite host rock | 5 | 40 | L/kg | uniform |
| KdDRZ | Cs $K_d$ in DRZ | 5 | 40 | L/kg | uniform |
| KdFrac | Cs $K_d$ in fracture | 5 | 40 | L/kg | uniform |

## RESULTS

Freeze et al. [2, 3] plotted color contours of $^{135}Cs$ concentration at $10^7$ y for two deterministic simulations of the stuck waste package scenario, with and without the lateral head gradient (Figure 3).

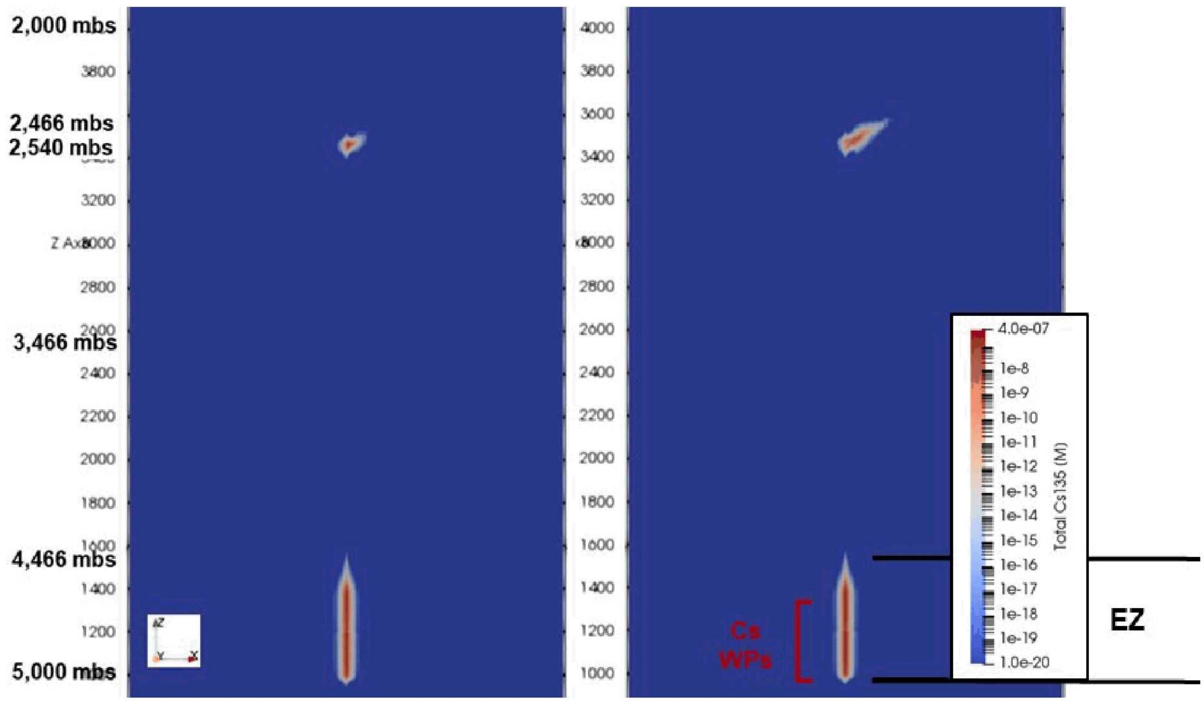


Figure 3. Dissolved concentration of $^{135}Cs$ at $10^7$ y for deterministic simulations [2].

This paper presents uncertainty and sensitivity analysis of $^{135}Cs$ concentrations at observation points in the cement plug and in the DRZ above the stuck waste package, and in the fracture to the east (downgradient) of the stuck waste package (Table II).

No analysis is presented of $^{137}Cs$ concentrations, which because of its short half-life, has completely decayed by 3000 y. Its concentration never increases above the initial condition at the observation points 50 m above the stuck waste package, nor at any of the observation points in the fracture.

TABLE II. Observation point distances from stuck waste package

| Cement Plug | Vertical Distance (m) | DRZ | Vertical Distance (m) | Fracture | Lateral Distance (m) |
|---|---|---|---|---|---|
| cem0 | 5 | drz0 | 5 | frac0 | 5 |
| cem1 | 25 | drz1 | 25 | frac1 | 25 |
| cem2 | 50 | drz2 | 50 | frac2 | 50 |
| cem3 | 75 | drz3 | 75 | frac3 | 100 |
| cem4 | 100 | drz4 | 100 | frac4 | 200 |

**Uncertainty**

The 200 predictions of $^{135}Cs$ concentration versus time at selected observation points are plotted in Figures 4 and 5. For reference, $^{135}Cs$ concentration versus time predicted by the deterministic simulation (heavy orange line) is plotted. Point-wise mean, median, and $5^{th}$ and $95^{th}$ percentiles are also shown.

In the cement plug, concentrations of $^{135}Cs$ reach peak values between $10^{-12}$ and $10^{-8}$ mol/L at a distance of 25 m above the stuck waste package, as high as $10^{-13}$ mol/L 50 m above the stuck waste package, and increase above the initial condition in only a handful of simulations 75 m above the stuck waste package (Figure 4). Concentrations in the DRZ at adjacent observation points (not shown) are nearly identical to concentrations in the cement plug.

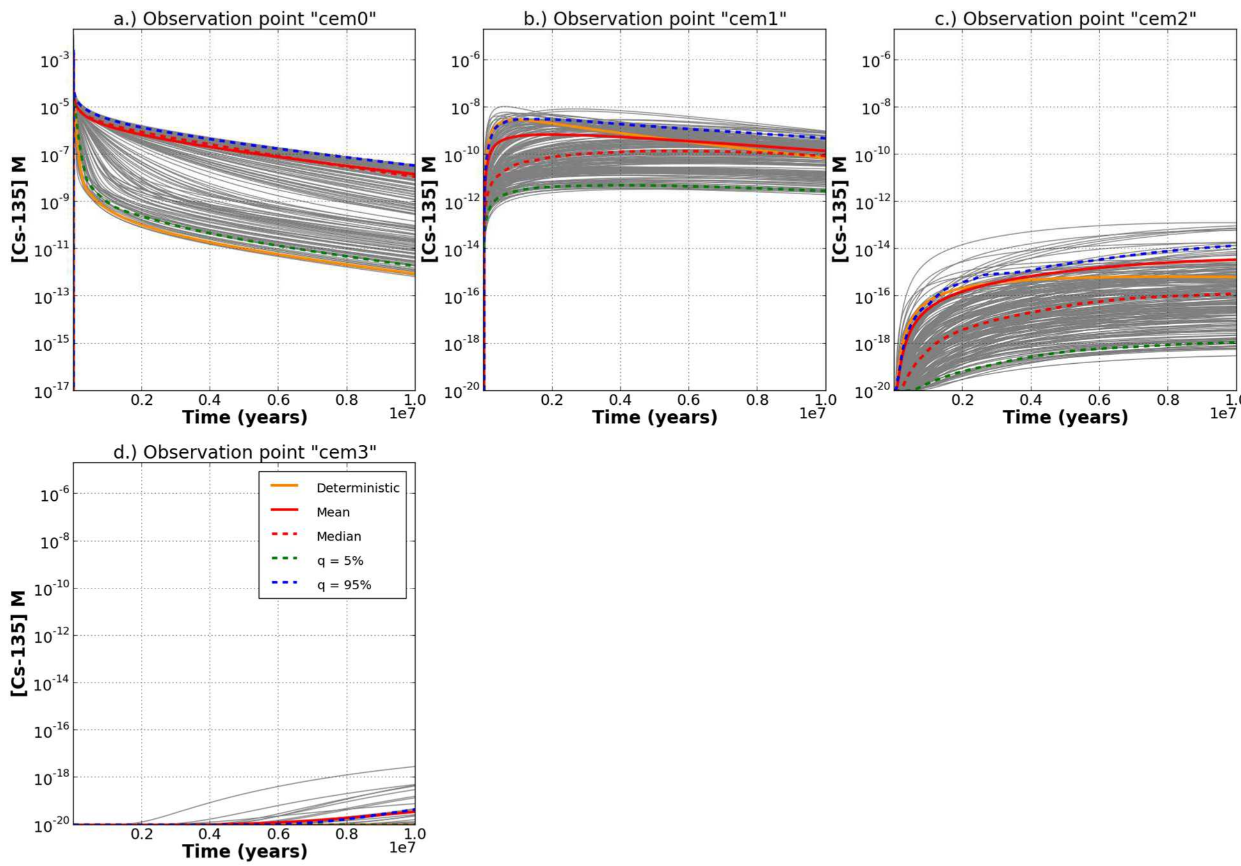


Figure 4. Concentration of $^{135}Cs$ versus time at observation points in the cement plug above the stuck waste package. Vertical axis limits in (a) are larger than in (b – d).

In the fracture zone, concentrations of $^{135}Cs$ reach peak values between $10^{-8}$ and $10^{-5}$ mol/L five meters from the stuck waste package, and between $10^{-17}$ and $10^{-7}$ at a lateral distance of 25 m from the stuck waste package (Figure 5). At a lateral distance of 200 m, $^{135}Cs$ concentration does not rise above initial conditions in any simulation until after $10^{6}$ y, the median concentration never rises above initial conditions, and all but four simulations predict peak concentrations $<10^{-10}$ mol/L (Figure 5e).

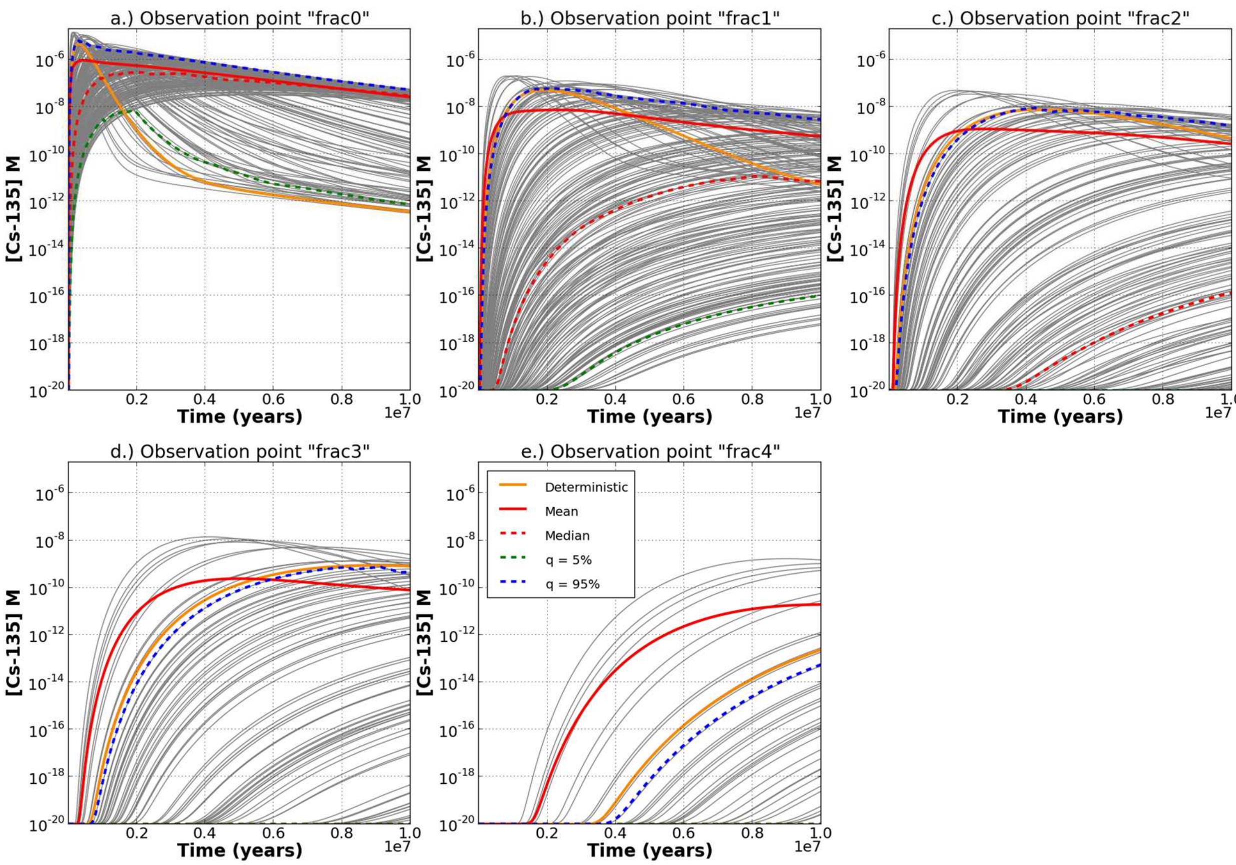


Figure 5. Concentration of $^{135}$Cs versus time at observation points in the fracture, downgradient of the stuck waste package.

**Sensitivity**

Scatter plots are used to visualize correlations between maximum $^{135}$Cs concentration (regardless of time) and sampled inputs (Figure 6). Partial correlation coefficients (PCC) and partial rank correlation coefficients (PRCC) are used to quantify the relationships between input and output variables (Figure 7). A PCC measures the strength of the linear relationship between two variables ($x$ and $y$) after the effects of other variables have been removed. It is defined as the correlation between the residuals resulting from the linear regression of $x_j$ with $x_{\sim j}$ and $y$ with $x_{\sim j}$, respectively, where the notation $x_{\sim j}$ means all $x$ except $x_j$ [8]. The calculation of PRCCs, in which the raw values of $x$ and $y$ are replaced with rank values, improves correlation when the relationship between variables is nonlinear but monotonic and decreases the influence of outliers.

From the scatter plots (Figure 6), it is evident that the maximum $^{135}$Cs concentration at most locations in both the cement plug and the fracture increases with increasing fracture permeability (kFrac), and decreases with increasing sorption coefficient (KdFrac). Breach time, and cement plug porosity and permeability influence maximum concentration in the cement plug 5 m above the stuck waste package (top row). Increasing the sorption coefficient in the granite host rock decreases the maximum concentration in the cement plug further from the waste package.

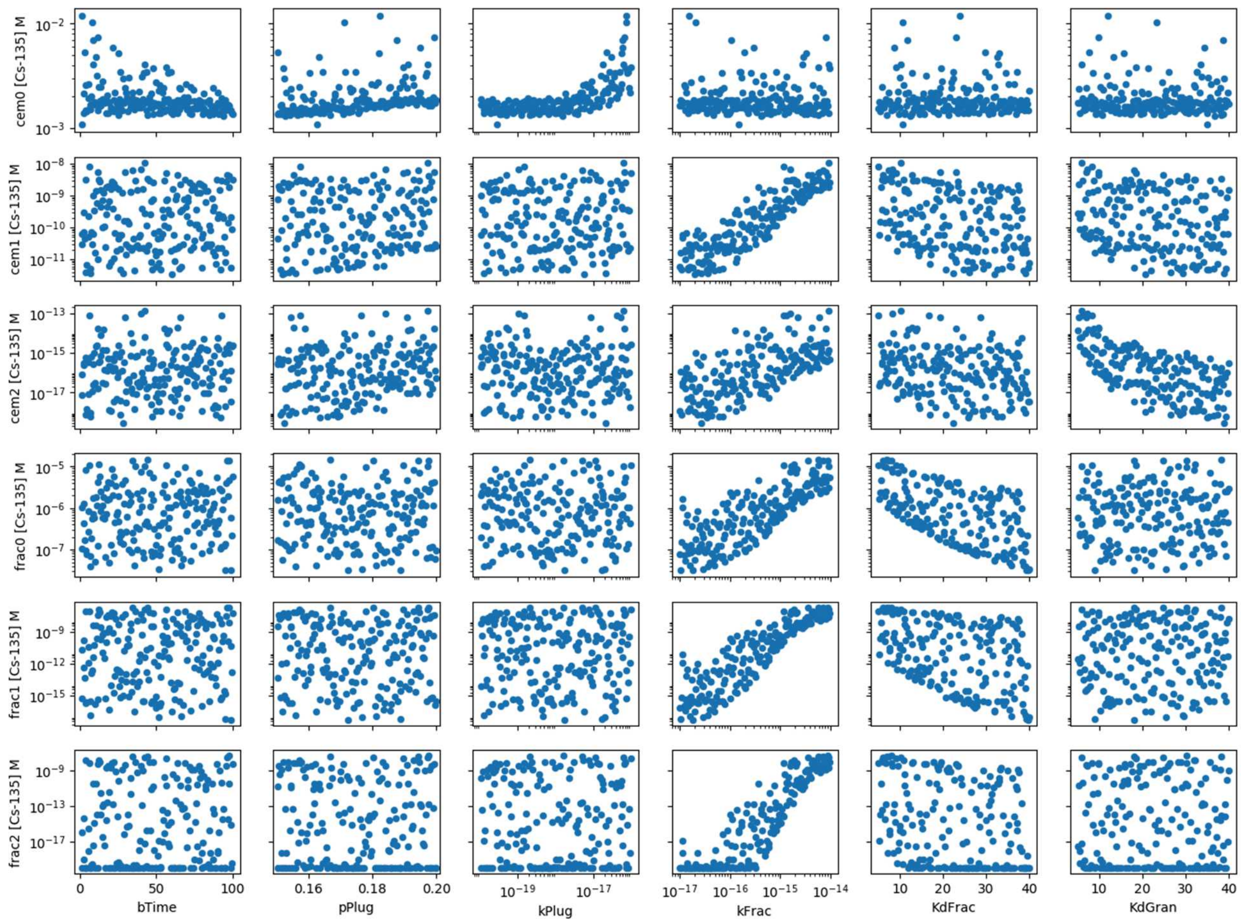


Figure 6. Selected scatter plots of maximum $^{135}$Cs concentration versus sampled inputs.

PCCs and PRCCs quantify these relationships; a PCC or PRCC with an absolute value of approximately 0.2 is statistically significant with a p-value of 0.05. In the cement plug immediately above the stuck waste package (Figure 7a), maximum $^{135}$Cs concentration is positively correlated with plug porosity ($PCC_{pPlug}$ = 0.25) and plug permeability ($PCC_{kPlug}$ = 0.74), which influence diffusive and advective fluxes, respectively; and negatively correlated with waste package breach time ($PCC_{bTime}$ = -0.46). At observation points higher in the cement plug (Figures 7b and 7c), maximum $^{135}$Cs concentration is not sensitive to properties of the cement plug. Instead, it is positively correlated with fracture permeability and negatively correlated with sorption coefficients in the fracture zone and in the granite host rock; 25 m above the stuck waste package these correlations are $PCC_{kFrac}$ = 0.75, $PCC_{KdFrac}$ = -0.47, and $PCC_{KdGran}$ = -0.30.

At observation points in the fracture, peak concentration of $^{135}$Cs is positively correlated with fracture permeability and negatively correlated with the sorption coefficient in the fracture zone. Five meters east of the stuck waste package $PCC_{kFrac}$ = 0.73 and $PCC_{KdFrac}$ = -0.62; PRCCs are larger. The strength of these correlations as measured by PCC decreases with distance from the stuck waste package; the correlation as measured by PRCC remains strong.

In these simulations, the fracture zone provides a high-permeability conduit whose properties influence concentrations in the cement plug tens of meters above the stuck waste package as well as in the fracture itself.

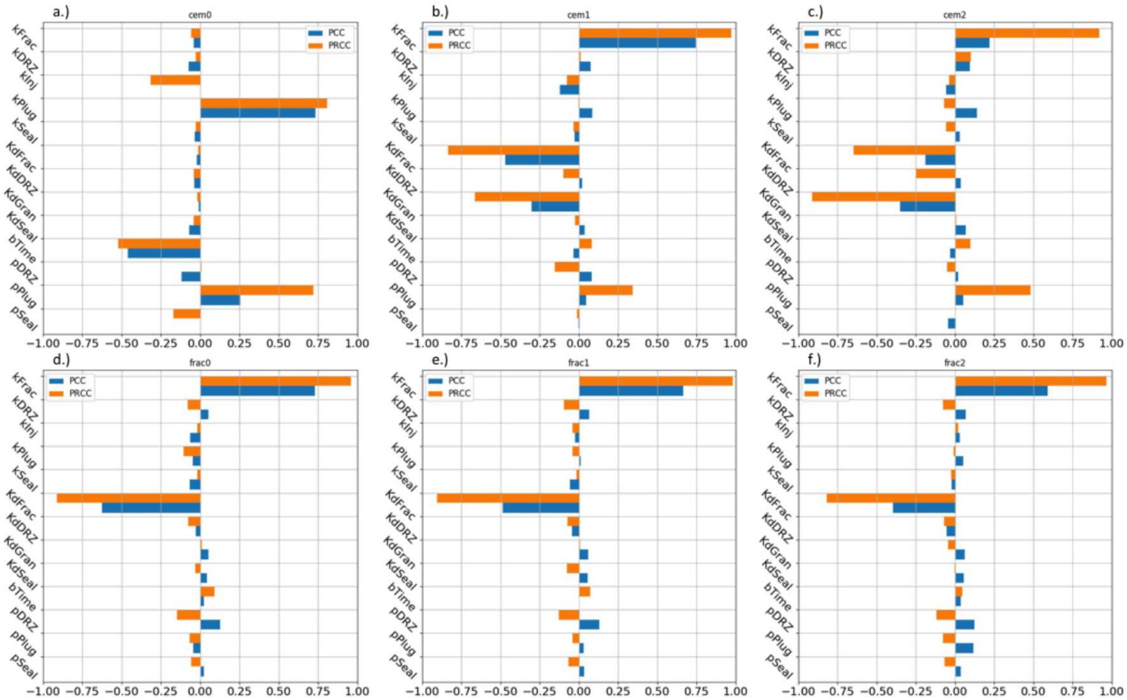


Figure 7. PCC and PRCC relating maximum $^{135}Cs$ concentration to sampled inputs at observation points in the cement plug and in the fracture zone.

## CONCLUSION

This paper builds upon previous work by Freeze et al. [1, 2, 3] to present a probabilistic PA of the stuck waste package scenario. Uncertainties affecting radionuclide mobilization and transport are propagated through 200 realizations of a subsurface flow and transport model to quantify uncertainties in predicted radionuclide concentrations within the borehole and the fracture zone. Simulations predict no radionuclide transport in the borehole at distances greater than 100 m above the stuck waste package. The assumed lateral pressure gradient of 0.0001 m/m leads to limited advective transport in the transmissive fracture zone. None of the simulations predict radionuclide transport to a lateral distance of 200 m from the stuck waste package at times less than $10^6$ y; fewer than half of the simulations predict radionuclide transport to this distance by $10^7$ y. In both the borehole and the fracture, peak concentrations are sensitive to fracture permeability and sorption coefficient. These results complement previous results for the nominal scenario and contribute to the development of a generic safety case for DBD.

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## ACKNOWLEDGEMENTS

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