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Numerical Modeling of Contaminant Transport from Grouted Residual Waste in the 221-U Facility (U Plant)

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1.0 Introduction

This letter report documents the numerical analyses conducted by Pacific Northwest National Laboratory (PNNL) to provide support for a feasibility study on decommissioning the 221-U canyon building at Hanford. The 221-U facility is the first of the major canyon buildings to be decommissioned. The specific objective of this modeling effort was to assess the potential for water penetration and leaching of contaminants from the grouted canyon structure and its subsequent transport through the vadose zone into groundwater during the first 1,000 years after the canyon is grouted and the roof and the walls above deck level are demolished (Gibson 2005). To evaluate the effects of installing an environmental cap, two cases, one with and one without the cap, were simulated.

A previous modeling effort (Rockhold et al. 2004), which was conducted on a small domain, that is, the grouted canyon monolith only, and for a short time period (up to 40 years) after the decommissioning, was used as a base model in this current modeling effort. The current modeling domain was extended from that of previous modeling both horizontally and vertically, adding the appropriate geological strata between the surface and groundwater as needed. The effects of the environmental cap on water infiltration and contaminant transport at the canyon deck was simulated by adjusting the water recharge rate at the soil surface. The recharge rates used in this modeling differ from the previous study because of the significantly longer time frame of interest. A higher recharge rate through the barrier was assumed to conservatively bound potential barrier performance and weather variations. While recent evapotranspiration barrier test data indicate that a recharge rate approaching 0.1 mm/yr may be achieved, a rate of 0.5 mm/yr was used for this study. The rate was increased by a factor of 2 after 500 years to reflect the possibility of barrier degradation.

The information is expected to assist in the responsiveness summary for the U-Plant Proposed Plan, providing an evaluation of the effectiveness of the proposed preferred alternative for the longer term and demonstrating the potential need for an environmental cap. The primary concern is the transport of the contaminants through the vadose zone to groundwater. The purpose of this effort was to determine whether contaminants will reach groundwater and, if so, what concentration level would impact the groundwater.

This report is organized as follows. A brief description of the canyon buildings and the activity involved is given, although the history of the canyon buildings at Hanford and a summary of recent characterization activities at the 221-U facility are described in Jacques (2001, p.2-1) and Rockhold et al. (2004). Simulations of contaminant transport were conducted using the STOMP numerical flow simulator. A brief description of the STOMP is given below. Section 2 contains a discussion of the physical, hydraulic, and transport properties and model parameters that were used to represent the engineered materials and sediments around the facility, and the geological units in the vadose zone. The modeling assumptions, grid specifications, and boundary and initial conditions are then described. The simulation results are presented in Section 3, followed by discussion and conclusions. Cited references are included in Section 4. The assumed initial radionuclide inventories and the physical, hydraulic, and transport parameters that were used in the modeling are tabulated in the appendixes.

1.1 U-Plant

U-Plant (221-U facility), located in the 200 West Area, is one of the five canyon buildings on the Hanford Site. U-Plant was constructed in the early to mid-1940s in support of World War II plutonium production. These buildings are referred to as "canyon buildings" because of their immense size and the canyon-like appearance of their interiors.

The U Plant, together with B Plant and T Plant, were originally designed as bismuth-phosphate chemical separations plants to extract plutonium from fuel rods irradiated in Hanford's production reactors, but it was never actually used for this purpose because the capacities of the B and T Plants were apparently sufficient to meet production goals. In 1952 it was converted to the tributyl phosphate (TBP) process to recover uranium from high-level bismuth-phosphate wastes. It was placed in standby mode in 1958 and was subsequently retired. All TBP process hardware was cleaned in 1957 and remains in place. Decontamination and reclamation activities took place in the building from 1958 to 1964. The building is now inactive and contains legacy equipment. The focus of the current study is the decommissioning of the 221-U facility.

1.2 Description of the STOMP Simulator

Numerical simulations of contaminant transport from the 221-U facility were conducted using the STOMP simulator (White and Oostrom 2003). STOMP is a numerical model that simulates heat and mass transfer through multiple fluid phases in porous media systems. STOMP is currently used to support several different performance and risk assessment activities across the Hanford Site (e.g., tank farm field investigation, etc.) and has undergone extensive testing and verification with comparisons of simulation results to analytical solutions and laboratory and field data (http://www.pnl.gov/etd/stomp/).

Mode 1 of STOMP was used in this work. This mode solves a single governing equation for the mass balance of liquid water under isothermal conditions, and separate mass balance equations for the advection and diffusion/dispersion of aqueous-phase solutes. Complete descriptions of the governing equations and numerical methods used in STOMP are given by White and Oostrom (1996).

2.0 Modeling Assumptions and Initial and Boundary Conditions

Two types of information were needed to execute the STOMP simulator, including 1) a simulation control and material definition and 2) soil zonation. The soil zonation denotes the rock/soil type for every grid cell in the computational domain, which was defined by the decommissioning process expected in the canyon building and the geological units between the surface and the water table. The decommissioning involves cutting the roofs off the canyon buildings; entombing the process cells, piping and electrical galleries, drains, and any residual contamination that may be contained in the buildings with grout; and then placing infiltration barriers over them. The focus of previous modeling effort was on the near-field system, so surface infiltration barriers and most of the vadose zone and underlying aquifer were not included in that analysis. The current modeling effort assesses the potential of water penetration and leaching of contaminants from the grouted canyon structure and their subsequent transport through the vadose zone into the groundwater.

It was assumed, as it was in the previous modeling, that the concrete structure of the facility contains no significant cracks or other features that could lead to preferential movement of percolating water through the waste and out of the facility into the surrounding environment. For further discussion on estimating cracks for the grout vault engineered barriers, please refer to Appendix Q of Kincaid et al. (1995).

Figure 1 shows the two-dimensional cross section of the 80 × 83-m simulation domain. The small rectangular part in the top center of the simulation domain is the canyon building to be grouted, with dimensions of 66.25 ft (20.2 m) by 34 ft (10.36 m). The size and location of the concrete structure of the building and the facilities to be grouted can be seen clearly from an enlarged view of the grouted canyon monolith shown in Figure 2. As in the previous modeling effort, buffer regions 10.36 m wide were included on either side of the facility to account for backfilled soil materials that were put in place after its initial construction (above sloping lines in Figures 1 and 3). A 30-cm-thick compacted soil material was designated for the region immediately under the facility to represent compacted sediments underlying the structure. A 1-m-thick region spanning the top of the model domain was assigned properties of Hanford gravel to allow for diversion of infiltrating water across the top of the underlying concrete structure. The entire simulation domain was extended from this subdomain both horizontally and vertically. Horizontally, the domain was extended another 20 m on each side of the buffer zones and vertically extended from the surface through the vadose zone to the water table. The depths of the geologic units in the rest of the domain are shown in Figure 1. The physical and hydraulic properties of the engineering material of the subdomain (including the grouted canyon monolith and the backfill buffer region) were given the values used in previous modeling (Rockhold et al. 2004), and the physical and hydraulic properties of the geological units were obtained from the 'vadose zone hydrogeology data package for the 2004 composite analysis (Last et al. 2004). This data package describes the geologic framework; the physical, hydrologic, and contaminant transport properties of the geologic materials; and deep drainage estimates building on the general framework developed for the initial assessment conducted using the System Assessment Capability (SAC). It is a compilation of the available data to support a composite analysis of Hanford's impact. The properties of the engineering materials and the geological units of the simulation domain are tabulated in Tables B.1 and B.2 of Appendix B.

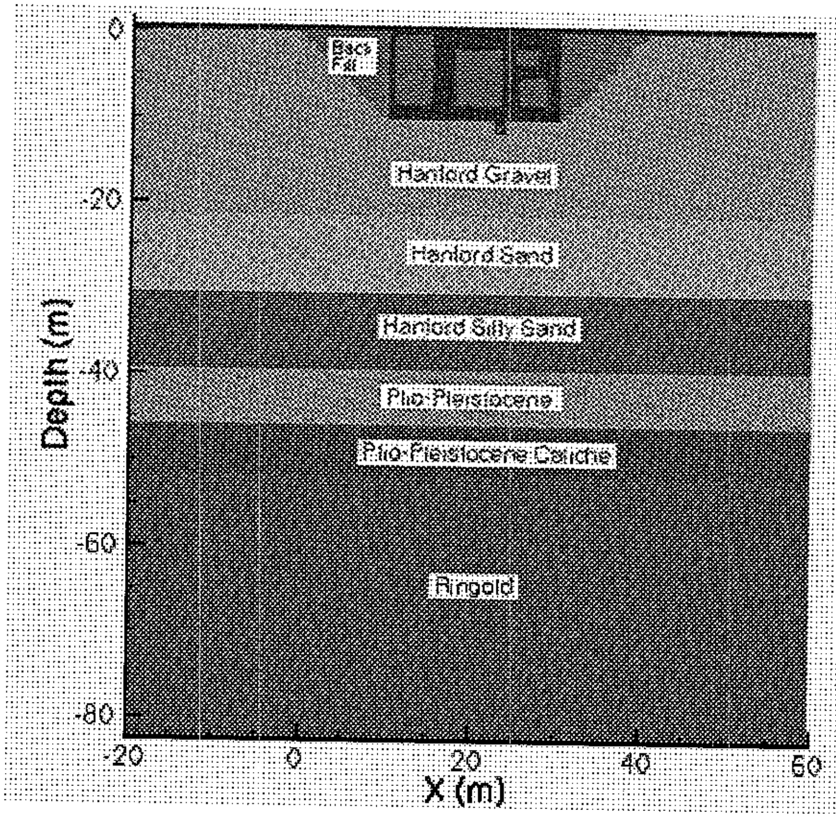

Figure 1. The Geological Units of the Simulation Domain

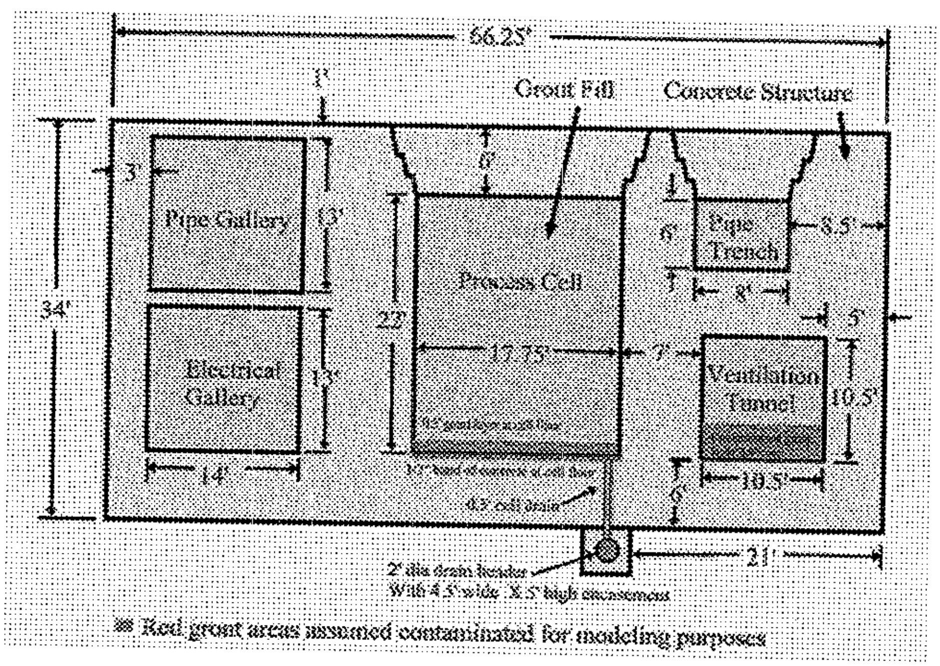

Figure 2. Representative Cross Section Through Decommissioned 221-U Facility Showing Physical Dimensions and Assumed Location of Contaminants

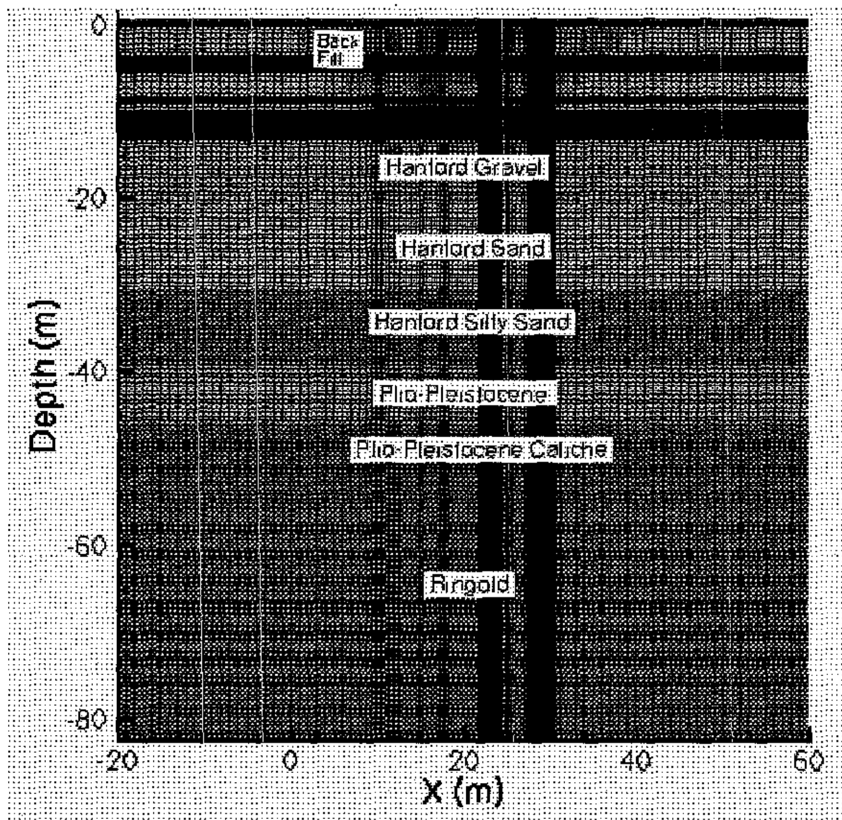

Figure 3. STOMP Model Grid for the Simulation Domain

In addition to the physical dimensions and the assumed locations of the decommissioning facilities, Figure 2 also shows the locations of the residual contamination of the 221-U facility after decommissioning (figure provided by Mark Gibson, FHC). An assumed radionuclide inventory was established for use as initial conditions in the modeling based on values obtained from the final 221-U facility characterization report (Jacques 2001). Four areas of residual contamination are depicted in Figure 2 and tabulated in Table 1. They include 1) a 6-inch-thick layer of grout in the bottom of the process cell, representing the first lift of poured grout and residuals at the bottom of vessels/equipment; 2) a ½-inch-thick layer of contaminated concrete at the base of the process cell underlying the grout; 3) a 2.6-ft-thick layer of grout in the bottom of the ventilation tunnel; and 4) a 2-ft-diameter drain header underneath the facility. The assumed inventory in these four areas was provided in a spreadsheet by Mark Gibson (FHC) and was based on the data reported by Jacques (2001). The initial radionuclide inventories are given in Tables A.1 through A.4 of Appendix A. To provide additional information on the potential transport of an extremely mobile contaminant in this modeling scenario, a unit value of ^{129}I was also included in the input data. This radionuclide is not considered a contamination of concern for the 221-U Facility in the CERCLA documentation and was analyzed for comparative purposes only.

The simulation domain was gridded as 149 by 233 computational nodes. The gridding of the simulation domain was based on the gridding strategy used on the subdomain of previous simulation (Rockhold et al. 2004). Specifically, the gridding of the subdomain was kept exactly the same as in previous modeling. As shown in Figure 3, the nodes spacing of the subdomain varies, ranging from 1.27

to 60.96 cm in the vertical direction and from 5 to 100 cm in the horizontal direction, with the finest discretization at the base of the grouted process cells and in the region representing the drain header. The regions of continuous black color in Figure 3 are areas where the grid is more finely discretized. The circular, 2-ft-diameter drain header depicted in Figure 2 was represented in the model as a rectangular, 0.551 by 0.554-m region with approximately the same cross-sectional area as the drain header. For the rest of the area outside the subdomain, a constant 100-cm horizontal spacing and a constant 50-cm vertical spacing are used.

The top boundary conditions used in the two simulation cases are as follows:

- Case 1 (with an environmental cap):
  - From 0 to 500 years, recharge rate = 0.5 mm/yr
  - From 500 to 1000 years, recharge rate = 1.0 mm/yr
- Case 2 (without an environmental cap)
  - From 0 to 1000 years, recharge rate = 43.1 mm/yr

Table 1. Source Areas

Source	Location
1	6-inch-thick layer of grout in the bottom of the process cell
2	½-inch-thick layer of contaminated concrete at the base of the process cell underlying the grout
3	2.6-ft-thick layer of grout in the bottom of the ventilation tunnel
4	2-ft-diameter drain header underneath the facility

The time-varying surface charge of cases 1 and 2 required a transient flow simulation to be executed with the solute transport calculation. Based on similar approaches used in the simulation of C, S-SX and T-TX-TY tank farms (Zhang et al. 2003, 2004a,b), the transient flow and transport simulations were initiated using a steady flow simulation to the boundary value problem with initial boundary values. This approach neglects time variations in surface recharge prior to the start of the simulation. The results of a steady-state run at the recharge rate, 3.5 mm/yr, were used as the initial condition of the two simulations. Note that the previous model, because it represented a much smaller physical size and a much shorter time frame, did not use these initial conditions but instead assumed specific soil moisture tension values. The lateral boundaries were specified as no-flow boundaries for water and solutes. The bottom boundary was specified as a zero tension (water table) boundary for water and an outflow boundary for solutes.

2.1 Hydraulic and Transport Properties

The constitutive permeability-saturation-capillary pressure relations for the materials in this study were represented by the following functions (van Genuchten 1978, Mualem 1976):

$$\theta = \theta_r + (\theta_s - \theta_r)\left[1 + (\alpha h)^n\right]^{-m} \qquad [1]$$

where θ is the volumetric water content, θ_s is the saturated water content or porosity, θ_r is the residual or irreducible water content, α, *n*, and *m* are empirical fitting parameters, and *h* is the soil-moisture tension, which is related to the capillary pressure. Unsaturated hydraulic conductivity was described by

$$K = K_s \frac{\left\{1-(\alpha h)^n\left[1+(\alpha h)^n\right]^{-m}\right\}^2}{\left[1+(\alpha h)^n\right]^{m/2}} \qquad [2]$$

where K_s is the hydraulic conductivity of the porous media when completely filled with water, and $m = 1 - 1/n$.

For the subdomain used in previous simulation parameters representing the physical and hydraulic properties of the backfill soil compacted soil under the facility and the building concrete were taken from previous modeling (Rockhold et al. 2004). The physical and hydraulic properties of the geological units surrounding the subdomain were taken from the SAC data package (Last et al. 2004).

Effective aqueous-phase diffusion coefficients were estimated from (Kemper and van Schaik 1966):

$$D_e(\theta) = D_{ab} a \exp(b\theta) \qquad [3]$$

where D_{ab} is the diffusion coefficient for the species in water, and *a* and *b* are empirical parameters. Diffusion and sorption coefficients for the natural and engineered materials were taken from Kincaid et al. (1995; Tables 3.14 and 3.15). Half-lives, $t_{1/2}$, for the radionuclides of interest were used the same values as in previous modeling (Rockhold et al. 2004), which in turn were taken from Lide (1996). Half-lives and diffusion and sorption coefficients are listed in Tables B.3 to B.7 of Appendix B.

3.0 Results and Discussion

The primary objective of this study was to estimate the rate of radionuclide migration out of the 221-U facility into the surrounding soil environment and its transport through the vadose zone to the water table. All of the radionuclides that were modeled are expected to adsorb to varying extents in the grout and concrete, as indicated by the assigned K_d values given in Tables B.4 and B.5. The simulated mass fractions of the total inventory of each radionuclide in grout, concrete, and soil are summarized in Tables 2a and 2b for 0 (initial condition), 100, 500 and 1000 years. These results indicate that, under the simulated conditions, the majority of most of the radionuclides that are known to be part of the inventory (Jacques 2001) remained in the grout but a fair amount of the radionuclides do diffuse out of the grout and into the surrounding concrete. While most of the radionuclides remained in the grout and the surrounding concrete during 1000 years, there were some exceptions. Two radionuclides with short half lives, ^{60}Co and ^{154}Eu, decayed out before they migrated out from the grout and concrete structure.

For informational purposes only, the movement of ^{129}I, which is not absorbed by soil particles, was also simulated. It is the only radionuclide that was transported out of the grout and concrete and into deeper sediments in any significant quantity during a long time period. Without an environmental cap, a significant portion of ^{129}I or other long-lived and extremely mobile radionuclide, if present, could reach the Ringold sediment after 1000 years.

The shortest distance between any of the contaminated areas and the soil environment outside of the concrete structure of the facility is around the drain header. If diffusion is the dominant mechanism for contaminant transport out of the facility, the soil environment around the drain header is likely to become contaminated before other areas. Figure 4a-c and Figure 5a-c depict simulated concentration distributions in the vicinity of the drain header for ^{137}Cs and ^{239}Pu at times of 0, 100, and 1000 years with (left) and without (right) an environmental cap. There is no visible difference between the contaminants concentration distributions for the two cases. This indicates that including the environmental barrier or not had little effect on the migration of the contaminants. The rate of migration of ^{137}Cs out of the grout is greater than that of ^{239}Pu due to the differences in K_d values (see Table B.5). One of the motivations for this modeling effort was to evaluate the effects of an environmental cap on the possible reduced transport of contaminants from the facility. Figures 4 and 5 clearly show that the addition of an environmental cap does not provide much difference in the contaminant transport for these contaminants over the time frame of interest.

Figure 6 depicts the streamline and aqueous saturation distributions at after 1000 years, with and without an environmental cap. It is clear that the aqueous saturation was higher when no environmental cap was used. However, the flow lines were almost the same for the two cases. Due to the low hydraulic conductivity of the concrete, recharge water was diverted to the sides of the concrete structure. Consequently, the contaminants within the grout and concrete did not migrate much.

The quantity of contaminants entered into the groundwater was also tracked. After 1000 years, for the case without an environment cap the percentage of contaminants that entered into groundwater was 57.6% for ^{129}I but zero for all the other contaminants; for the case with an environment cap, none of the contaminants entered into the groundwater.

Table 2a. Mass Fraction of Total Inventory Contained in Grout, Concrete, and Different Geological Units (with an environmental cap)

Year	Solute	Surface Gravel	Hanford Gravel	Concrete	Grout	Backfill	Compacted Soil	Hanford Sand	Hanford Silty Sand	Plio-Pleistocene	PP Caliche	Ringold
0	Eu154	0	0	0.00	100.00	0	0	0	0	0	0	0
0	Th230	0	0	100.00	0.00	0	0	0	0	0	0	0
0	Th232	0	0	0.00	100.00	0	0	0	0	0	0	0
0	Pu238	0	0	0.00	100.00	0	0	0	0	0	0	0
0	Pu239	0	0	0.00	100.00	0	0	0	0	0	0	0
0	Pu240	0	0	0.00	100.00	0	0	0	0	0	0	0
0	Am241	0	0	0.00	100.00	0	0	0	0	0	0	0
0	Co60	0	0	0.00	100.00	0	0	0	0	0	0	0
0	Sr90	0	0	0.00	100.00	0	0	0	0	0	0	0
0	Cs137	0	0	0.00	100.00	0	0	0	0	0	0	0
0	Np237	0	0	4.19	95.81	0	0	0	0	0	0	0
0	U234	0	0	0.00	100.00	0	0	0	0	0	0	0
0	U235	0	0	0.00	100.00	0	0	0	0	0	0	0
0	U238	0	0	0.00	100.00	0	0	0	0	0	0	0
0	I129	0	0	2.68	97.32	0	0	0	0	0	0	0
100	Eu154	0	0	0.07	99.93	0	0	0	0	0	0	0
100	Th230	0	0	98.52	1.48	0	0	0	0	0	0	0
100	Th232	0	0	0.13	99.87	0	0	0	0	0	0	0
100	Pu238	0	0	0.07	99.93	0	0	0	0	0	0	0
100	Pu239	0	0	0.07	99.93	0	0	0	0	0	0	0
100	Pu240	0	0	0.07	99.93	0	0	0	0	0	0	0
100	Am241	0	0	0.07	99.93	0	0	0	0	0	0	0
100	Co60	0	0	1.37	98.63	0	0	0	0	0	0	0
100	Sr90	0	0	1.37	98.63	0	0	0	0	0	0	0
100	Cs137	0	0	1.37	98.63	0	0	0	0	0	0	0
100	Np237	0	0	5.09	94.91	0	0	0	0	0	0	0
100	U234	0	0	0.13	99.87	0	0	0	0	0	0	0
100	U235	0	0	0.13	99.87	0	0	0	0	0	0	0
100	U238	0	0	0.13	99.87	0	0	0	0	0	0	0
100	I129	0	5.23	34.91	59.07	0.10	0.69	0.00	0	0	0	0
1000	Eu154	na	na	na	na	na	na	na	na	na	na	na
1000	Th230	0	0	87.34	12.66	0	0	0	0	0	0	0
1000	Th232	0	0	1.18	98.82	0	0	0	0	0	0	0
1000	Pu238	0	0	0.67	99.33	0	0	0	0	0	0	0
1000	Pu239	0	0	0.67	99.33	0	0	0	0	0	0	0
1000	Pu240	0	0	0.67	99.33	0	0	0	0	0	0	0
1000	Am241	0	0	0.67	99.33	0	0	0	0	0	0	0
1000	Co60	na	na	na	na	na	na	na	na	na	na	na
1000	Sr90	0	0	10.64	89.36	0	0	0	0	0	0	0
1000	Cs137	0	0	10.64	89.36	0	0	0	0	0	0	0
1000	Np237	0	0	10.11	89.89	0	0	0	0	0	0	0
1000	U234	0	0	1.18	98.82	0	0	0	0	0	0	0
1000	U235	0	0	1.18	98.82	0	0	0	0	0	0	0
1000	U238	0	0	1.18	98.82	0	0	0	0	0	0	0
1000	I129	0	21.49	37.35	34.33	1.02	1.39	4.36	0.06	0.00	0.00	0

na = the radionuclide has decayed to the level beyond detection.

Table 2b. Mass Fraction of Total Inventory Contained in Grout, Concrete, and Different Geological Units (without an environmental cap)

Year	Solute	Surface Gravel	Hanford Gravel	Concrete	Grout	Backfill	Compacted Soil	Hanford Sand	Hanford Silty Sand	Plio-Pleistocene	PP Caliche	Ringold
0	Eu154	0	0	0	100.00	0	0	0	0	0	0	0
0	Th230	0	0	100.00	0	0	0	0	0	0	0	0
0	Th232	0	0	0	100.00	0	0	0	0	0	0	0
0	Pu238	0	0	0	100.00	0	0	0	0	0	0	0
0	Pu239	0	0	0	100.00	0	0	0	0	0	0	0
0	Pu240	0	0	0	100.00	0	0	0	0	0	0	0
0	Am241	0	0	0	100.00	0	0	0	0	0	0	0
0	Co60	0	0	0	100.00	0	0	0	0	0	0	0
0	Sr90	0	0	0	100.00	0	0	0	0	0	0	0
0	Cs137	0	0	0	100.00	0	0	0	0	0	0	0
0	Np237	0	0	4.19	95.81	0	0	0	0	0	0	0
0	U234	0	0	0	100.00	0	0	0	0	0	0	0
0	U235	0	0	0	100.00	0	0	0	0	0	0	0
0	U238	0	0	0	100.00	0	0	0	0	0	0	0
0	I129	0	0	2.68	97.32	0	0	0	0	0	0	0
100	Eu154	0	0	0.07	99.93	0	0	0	0	0	0	0
100	Th230	0	0	98.57	1.43	0	0	0	0	0	0	0
100	Th232	0	0	0.13	99.87	0	0	0	0	0	0	0
100	Pu238	0	0	0.07	99.93	0	0	0	0	0	0	0
100	Pu239	0	0	0.07	99.93	0	0	0	0	0	0	0
100	Pu240	0	0	0.07	99.93	0	0	0	0	0	0	0
100	Am241	0	0	0.07	99.93	0	0	0	0	0	0	0
100	Co60	0	0	1.37	98.63	0	0	0	0	0	0	0
100	Sr90	0	0	1.37	98.63	0	0	0	0	0	0	0
100	Cs137	0	0	1.37	98.63	0	0	0	0	0	0	0
100	Np237	0	0	5.20	94.80	0	0	0	0	0	0	0
100	U234	0	0	0.13	99.87	0	0	0	0	0	0	0
100	U235	0	0	0.13	99.87	0	0	0	0	0	0	0
100	U238	0	0	0.13	99.87	0	0	0	0	0	0	0
100	I129	0	10.34	44.71	43.12	0.01	1.64	0.17	0.002213	1.87E-05	5.4E-07	1.59E-08
1000	Eu154	na	na	na	na	na	na	na	na	na	na	na
1000	Th230	0	0	87.81	12.19	0	0	0	0	0	0	0
1000	Th232	0	0	1.23	98.77	0	0	0	0	0	0	0
1000	Pu238	0	0	0.67	99.33	0	0	0	0	0	0	0
1000	Pu239	0	0	0.67	99.33	0	0	0	0	0	0	0
1000	Pu240	0	0	0.67	99.33	0	0	0	0	0	0	0
1000	Am241	0	0	0.67	99.33	0	0	0	0	0	0	0
1000	Co60	na	na	na	na	na	na	na	na	na	na	na
1000	Sr90	0	0	10.65	89.35	0	0	0	0	0	0	0
1000	Cs137	0	0	10.65	89.35	0	0	0	0	0	0	0
1000	Np237	0	0	10.89	89.11	0	0	0	0	0	0	0
1000	U234	0	0	1.23	98.77	0	0	0	0	0	0	0
1000	U235	0	0	1.23	98.77	0	0	0	0	0	0	0
1000	U238	0	0	1.23	98.77	0	0	0	0	0	0	0
1000	I129	0	10.88	16.72	12.59	0.02	1.16	7.09	9.24	5.22	4.51	32.5653

na = the radionuclide has decayed to the level beyond detection.

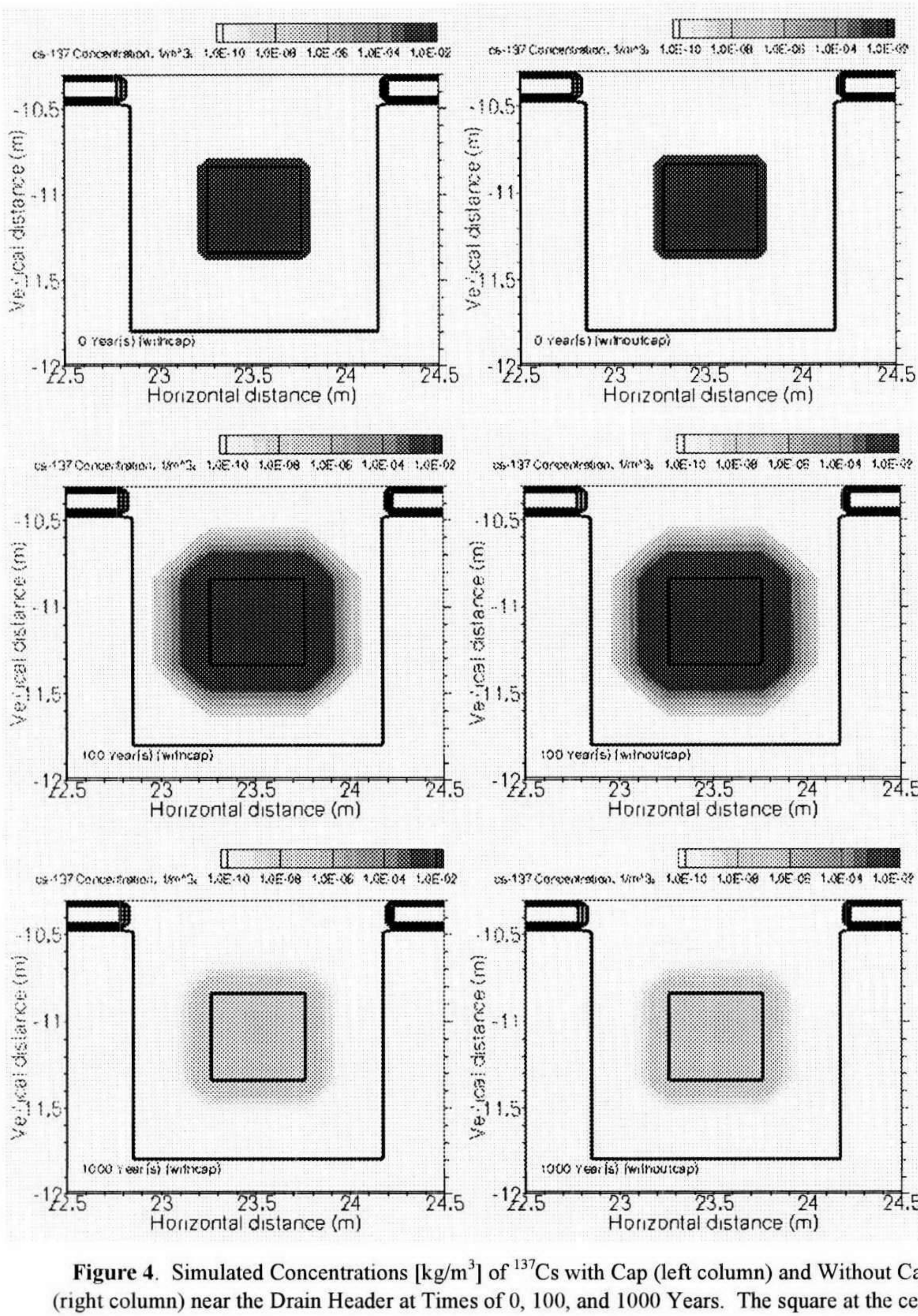

Figure 4. Simulated Concentrations [kg/m^3] of ^{137}Cs with Cap (left column) and Without Cap (right column) near the Drain Header at Times of 0, 100, and 1000 Years. The square at the center of each plot is the drain header.

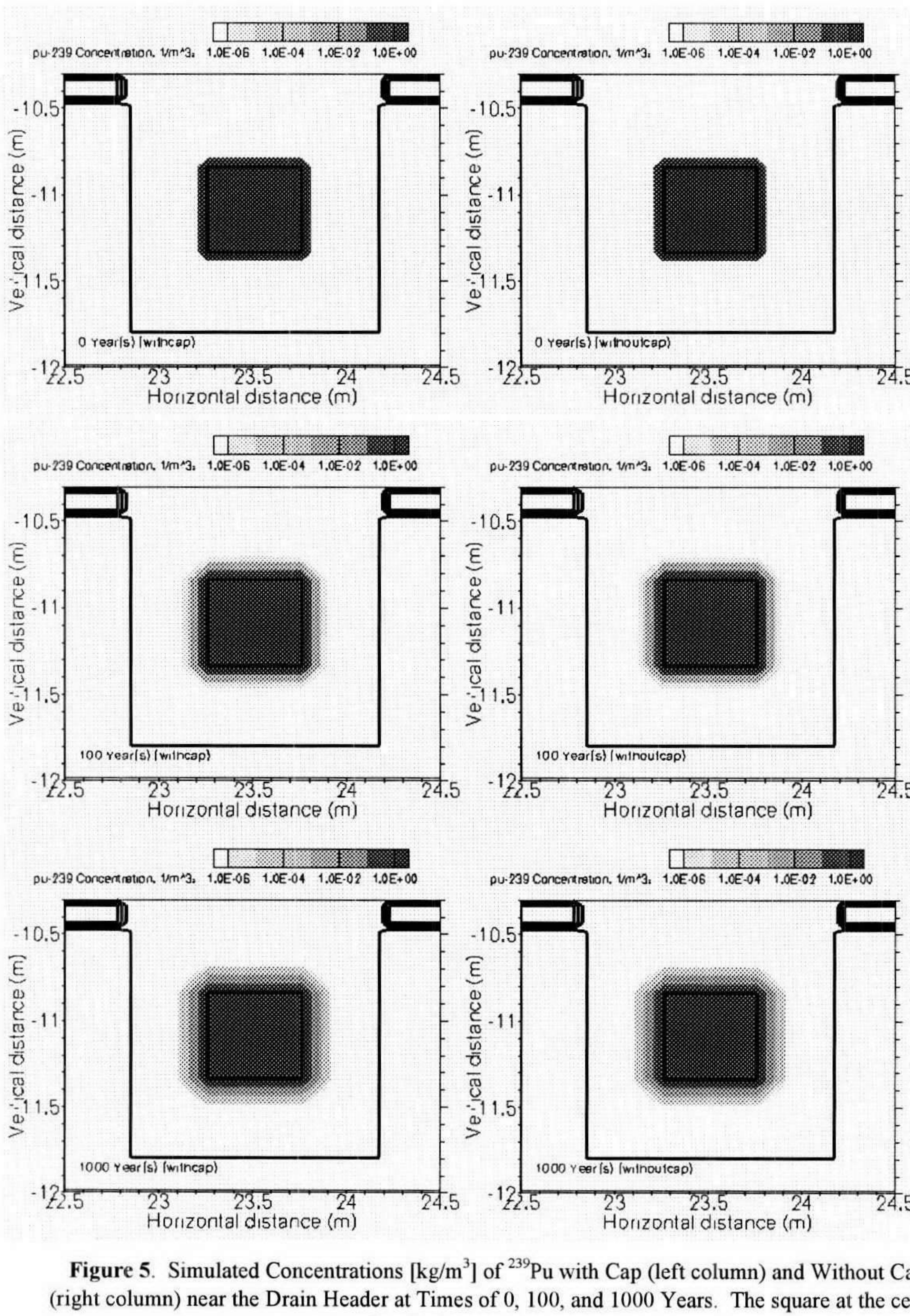

Figure 5. Simulated Concentrations [kg/m^3] of ^{239}Pu with Cap (left column) and Without Cap (right column) near the Drain Header at Times of 0, 100, and 1000 Years. The square at the center of each plot is the drain header.

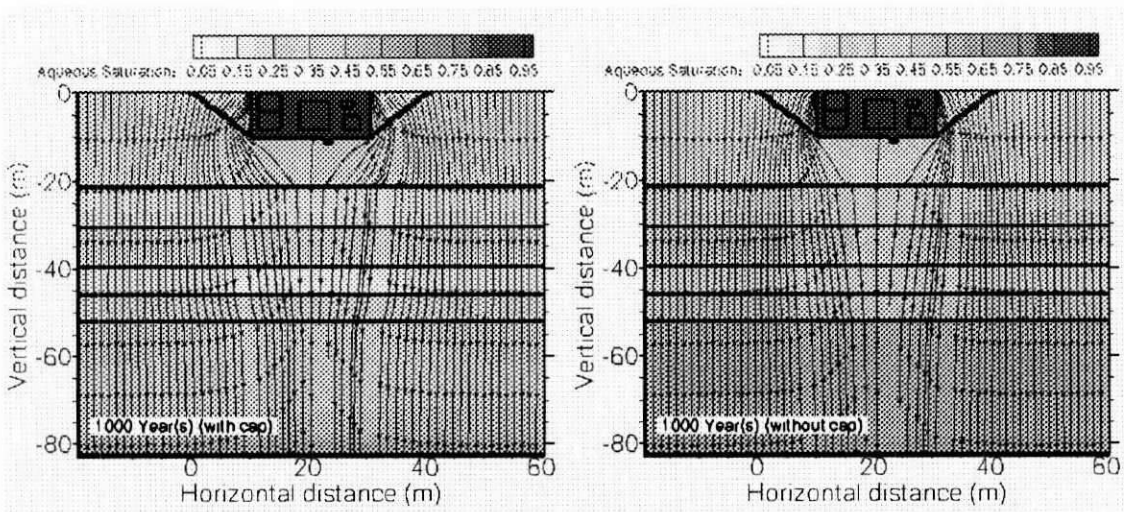

Figure 6. Simulated Streamlines and Soil Water Saturation Contours after 1000 Years for Cases with and Without an Environmental Cap above the U-Plant Monolith

In summary, the numerical simulations show that 1) the majority of radionuclides remain in the grout and the surrounding concrete within the 1000-year time frame and 2) for both cases, no radioactive contaminants of concern entered into the groundwater system after 1000 years.

The parameters used in the simulations no doubt had some uncertainties. The properties of concrete and grout had more dominant effects on the contaminant transport than the properties of other materials. It was assumed that there were no cracks in the concrete. Any occurrence of continuous crack/fracture will significantly affect the flow and transport of contaminants.

4.0 References

Gibson M. 2005. *Statement of Work: Perform Additional Computer Modeling of Grouted U Canyon Facility to Determine Water Movement and Contaminant Transport.* Fluor Hanford, Inc., Richland, Washington.

Jacques ID. 2001. Final data report for the 221-U facility characterization. BHI-01565, Rev. 0., Bechtel Hanford, Inc.

Kemper WD and JC van Schaik. 1966. "Diffusion of salts in clay-water systems." *Soil Sci. Am. Proc.*, 30:534-540.

Kincaid CT, JA Voodg, JW Shade, JH Westsik Jr, GA Whyatt, MD Freshley, MG Piepho, KA Blanchard, K Rhoads, and BG Lauzon. 1995. *Performance Assessment of Grouted Double-Shell Tank Waste Disposal at Hanford.* WHC-SD-WM-EE-004 Rev. 1, Westinghouse Hanford Company, Richland, Washington.

Last, GV, EJ Freeman, KJ Cantrell, MJ Fayer, GW Gee, WE Nichols, and BN Bjornstad. 2004. *Vadose zone hydrogeology data package for the 2004 composite analysis.* PNNL-14702 Rev 0, Pacific Northwest National Laboratory, Richland, WA.

Lide DR (ed.). 1996. *Handbook of Chemistry and Physics.* CRC Press, Inc., Boca Raton, Florida.

Mualem Y. 1976. "A New Model for Predicting the Hydraulic Conductivity of Unsaturated Porous Media." *Water Resources Research*, 12: 513-522.

Rockhold ML, MD White, and EJ Freeman. 2004. *Canyon Disposal Initiative—Numerical Modeling of Contaminant Transport from Grouted Residual Waste in the 221-U Facility (U-Plant).* PNNL-14908, Pacific Northwest National Laboratory, Richland, Washington.

van Genuchten MTh. 1978. *Mass transport in saturated-unsaturated media: One-dimensional solutions*, 78-WR-11, Princeton University, Princeton, New Jersey, p. 102.

White MD and M Oostrom. 1996. *STOMP—Subsurface Transport Over Multiple Phases, Theory Guide.* PNNL-11217, Pacific Northwest National Laboratory, Richland, Washington.

White MD and M Oostrom. 2003. *STOMP—Subsurface Transport Over Multiple Phases, Version 3.1, User's Guide.* PNNL-14478, Pacific Northwest National Laboratory, Richland, Washington.

Zhang, ZF, VL Freedman, and MD White. 2003. *2003 initial assessments of closure for the C tank farm: numerical simulations.* PNNL-14334. Pacific Northwest National Laboratory, Richland, Washington.

Zhang F, VL Freedman, SR Waichler, and MD White. 2004a. *Initial Assessments of Closure for the S-SX Tank Farm: Numerical Simulations.* PNNL-14604. Pacific Northwest National Laboratory, Richland, Washington.

Zhang, ZF, VL Freedman, and SR Waichler. 2004b. *2004 Initial Assessments for the T and TX TY Tank Farms Field Investigation Report (FIR): Numerical Simulations*. PNNL-14838. Pacific Northwest National Laboratory, Richland, Washington.

Appendix A

Radionuclide Inventories Used for Initial Conditions in STOMP Simulations

Appendix A - Radionuclide Inventories Used for Initial Conditions in STOMP Simulations

Table A.1. Assumed Initial Radionuclide Inventory in Process Cell Grout

Radionuclide	pCi/g	g/g	kg/m^3
^{60}Co	4.569E+05	4.039E-10	9.694E-07
$^{89/90}$Sr	4.351E+07	3.186E-07	7.647E-04
^{137}Cs	3.150E+07	3.645E-07	8.749E-04
^{154}Eu	2.559E+02	9.471E-13	2.273E-09
^{230}Th	0.000E+00	0.000E+00	0.000E+00
^{232}Th	3.227E+01	2.934E+04	7.041E-01
^{234}U	1.765E+04	2.832E-06	6.797E-03
^{235}U	6.185E+03	2.864E-03	6.874E+00
^{237}Np	2.095E-01	2.975E-10	7.140E-07
^{238}U	1.310E+05	3.893E-01	9.343E+02
^{238}Pu	1.197E+01	7.000E-13	1.680E-09
^{239}Pu	2.805E+05	4.526E-06	1.086E-02
^{240}Pu	2.242E+05	9.848E-07	2.364E-03
^{241}Am	2.209E+05	6.443E-08	1.546E-04

Table A.2. Assumed Initial Radionuclide Inventory in Process Cell Concrete Grout

Radionuclide	pCi/g	g/g	kg/m^3
^{60}Co	0.22	1.945E-16	4.785E-13
$^{89/90}$Sr	64600	4.731E-10	1.164E-06
^{137}Cs	60200	6.966E-10	1.714E-06
^{154}Eu	37	1.369E-13	3.368E-10
^{230}Th	64	3.107E-09	7.643E-06
^{232}Th	0	0	0
^{234}U	1.40	2.247E-10	5.527E-07
^{235}U	0.05	2.316E-08	5.696E-05
^{237}Np	0.13	1.846E-10	4.541E-07
^{238}U	1.60	4.754E-06	1.170E-02
^{238}Pu	22	1.286E-12	3.164E-09
^{239}Pu	224	3.613E-09	8.889E-06
^{240}Pu	96	4.216E-10	1.037E-06
^{241}Am	181	5.278E-11	1.298E-07

Table A.3. Assumed Initial Radionuclide Inventory in Ventilation Tunnel Grout

Radionuclide	pCi/g	g/g	kg/m^3
^{60}Co	0	0	0
$^{89/90}Sr$	11510	8.430E-11	2.023E-07
^{137}Cs	834.400	9.656E-12	2.317E-08
^{154}Eu	0	0	0
^{230}Th	0	0	0
^{232}Th	0	0	0
^{234}U	9.189E-01	1.475E-10	3.539E-07
^{235}U	6.337E-02	2.935E-08	7.044E-05
^{237}Np	2.693E-02	3.824E-11	9.177E-08
^{238}U	1.003	2.982E-06	7.156E-03
^{238}Pu	1.373E-01	8.026E-15	1.926E-11
^{239}Pu	7.171	1.157E-10	2.776E-07
^{240}Pu	3.073	1.350E-11	3.240E-08
^{241}Am	1.780	5.189E-13	1.245E-09

Table A.4. Assumed Initial Radionuclide Inventory in Drain Header Grout

Radionuclide	μg/g	kg/m^3
^{60}Co	5.800E+01	1.392E-01
$^{89/90}Sr$	1.489E+05	3.573E+02
^{137}Cs	6.839E+05	1.641E+03
^{154}Eu	1.353E+03	3.246E+00
^{230}Th	0	0
^{232}Th	0	0
^{234}U	0	0
^{235}U	0	0
^{237}Np	0	0
^{238}U	2.251E+01	5.402E-02
^{238}Pu	6.449E+01	1.548E-01
^{239}Pu	1.082E+03	2.596E+00
^{240}Pu	4.636E+02	1.113E+00
^{241}Am	7.488E+02	1.797E+00

Appendix B

Physical, Hydraulic, and Transport Parameters Used for STOMP Simulations

Appendix B - Physical, Hydraulic, and Transport Parameters Used for STOMP Simulations

Table B.1. Physical and Hydraulic Properties of Sediments and Engineered Materials (Rockhold et al. 2004) for the Disturbed Area at U Plant

Geologic Unit	Unit #	Depth (ft)	Depth (m)	ρ_b (g/cm^3)	ρ_p (g/cm^3)	θ_s (cm/cm^3)	K_s (cm/s^{-1})	α (cm^1)	n (-)	θ_r (cm/cm^3)	S_r (-)
Grout	1			2.4	2.63	0.087	1.47E-08	1.08E-05	1.65	0	0
Concrete	2			2.453	2.63	0.067	1.33E-09	3.87E-05	1.29	0	0
Surface Gravel	3			1.35	2.8	0.518	1.85	3.54	2.66	0.014	0.027
Compacted Soil	4			1.76	2.72	0.353	1.80E-06	0.0121	1.37	0.003	0.092
Backfill	5			1.889	2.76	0.316	1.91E-03	0.035	1.72	0.049	0.155

Table B.2. Physical and Hydraulic Properties of Geologic Units (Last et al. 2004, Appendix, Template S) for the Undisturbed Area at U Plant

Geologic Unit	Unit #	Depth (ft)	Depth (m)	ρ_b (g/cm^3)	ρ_p (g/cm^3)	θ_s (cm/cm^3)	K_s (cm/s^{-1})	α (cm^1)	n (-)	θ_r (cm/cm^3)	S_r (-)
Hanford Gravel	6	0-70	0-21.3	1.89	2.23	0.154	1.48E-03	1.65E-02	1.745	0.027	0.172
Hanford Sand	7	70-100	21.3-30.5	1.7	2.64	0.356	3.67E-05	1.02E-02	2.177	0.042	0.118
Hanford Silty Sand	8	100-130	30.5-39.6	1.67	2.77	0.398	1.91E-05	4.53E-03	2.116	0.057	0.141
Plio-Pleistocene	9	130-150	39.6-45.7	1.66	2.86	0.42	5.57E-05	5.52E-03	2.101	0.034	0.08
PP Caliche	10	150-170	45.7-51.8	1.71	2.46	0.306	5.00E-04	1.08E-02	1.727	0.072	0.214
Ringold	11	170-272	51.8-82.9	1.84	2.62	0.297	1.06E-04	1.32E-02	1.753	0.126	0.334
Aquifer		> 272	> 82.9	-	-	-	-	-	-	-	-

Table B.3. Atomic Weights and Half-Lives of Modeled Radionuclides

Radionuclide	Atomic Weight	$t_{1/2}$(yr)
Co-60	59.93	5.27
Sr-90	89.91	29.1
I-129		1.70E+07
Cs-137	136.91	30.2
Eu-154	153.92	8.59
Th-230	230.03	7.54E+04
Th-232	232.04	1.40E+10
U-234	234.04	2.45E+05
U-235	235.04	7.04E+08
Np-237	237.05	2.14E+06
U-238	238.05	4.46E+09
Pu-238	238.05	87.7
Pu-239	239.05	2.41E+04
Pu-240	240.05	6.54E+03
Am-241	241.06	4.32E+02

Table B.4. Diffusion and Sorption Coefficients for Soil Sediments

Radionuclide	K_d [m^3/kg]	D_{ab} [m^2/s]	*a*	*b*
Co-60	0.003	2.50E-09	0.005	10
Sr-90	0.003	2.50E-09	0.005	10
I-129	0	2.50E-09	0.005	10
Cs-137	0.003	2.50E-09	0.005	10
Eu-154	0.021	2.50E-09	0.005	10
Th-230	0.021	2.50E-09	0.005	10
Th-232	0.021	2.50E-09	0.005	10
U-234	0	2.50E-09	0.005	10
U-235	0	2.50E-09	0.005	10
Np-237	0.003	2.50E-09	0.005	10
U-238	0	2.50E-09	0.005	10
Pu-238	0.021	2.50E-09	0.005	10
Pu-239	0.021	2.50E-09	0.005	10
Pu-240	0.021	2.50E-09	0.005	10
Am-241	0.021	2.50E-09	0.005	10

Table B.5. Diffusion and Sorption Coefficients for Concrete

Radionuclide	K_d [m^3/kg]	D_{ab} [m^2/s]	*a*	*b*
Co-60	0.125	5.00E-12	1	0
Sr-90	0.125	5.00E-12	1	0
I-129	0	5.00E-12	1	0
Cs-137	0.125	5.00E-12	1	0
Eu-154	2.625	5.00E-12	1	0
Th-230	2.625	5.00E-12	1	0
Th-232	2.625	5.00E-12	1	0
U-234	2.625	5.00E-12	1	0
U-235	2.625	5.00E-12	1	0
Np-237	0.125	5.00E-12	1	0
U-238	2.625	5.00E-12	1	0
Pu-238	2.625	5.00E-12	1	0
Pu-239	2.625	5.00E-12	1	0
Pu-240	2.625	5.00E-12	1	0
Am-241	2.625	5.00E-12	1	0

Table B.6. Diffusion and Sorption Coefficients for Grout

Radionuclide	K_d [m^3/kg]	D_{ab} [m^2/s]	*a*	*b*
Co-60	0.125	1.00E-10	1	0
Sr-90	0.125	1.00E-10	1	0
I-129	0	1.00E-10	1	0
Cs-137	0.125	1.00E-10	1	0
Eu-154	2.625	1.00E-10	1	0
Th-230	2.625	1.00E-10	1	0
Th-232	2.625	1.00E-10	1	0
U-234	2.625	1.00E-10	1	0
U-235	2.625	1.00E-10	1	0
Np-237	0.125	1.00E-10	1	0
U-238	2.625	1.00E-10	1	0
Pu-238	2.625	1.00E-10	1	0
Pu-239	2.625	1.00E-10	1	0
Pu-240	2.625	1.00E-10	1	0
Am-241	2.625	1.00E-10	1	0

Table B.7. Diffusion and Sorption Coefficients for Surface Gravel

Radionuclide	K_d [m^3/kg]	D_{ab} [m^2/s]	*a*	*b*
Co-60	0.125	2.50E-14	0.005	10
Sr-90	0.125	2.50E-14	0.005	10
I-129	0	2.50E-14	0.005	10
Cs-137	0.125	2.50E-14	0.005	10
Eu-154	2.625	2.50E-14	0.005	10
Th-230	2.625	2.50E-14	0.005	10
Th-232	2.625	2.50E-14	0.005	10
U-234	2.625	2.50E-14	0.005	10
U-235	2.625	2.50E-14	0.005	10
Np-237	0.125	2.50E-14	0.005	10
U-238	2.625	2.50E-14	0.005	10
Pu-238	2.625	2.50E-14	0.005	10
Pu-239	2.625	2.50E-14	0.005	10
Pu-240	2.625	2.50E-14	0.005	10
Am-241	2.625	2.50E-14	0.005	10

Reference

Rockhold ML, MD White, and EJ Freeman. 2004. *Canyon Disposal Initiative—Numerical Modeling of Contaminant Transport from Grouted Residual Waste in the 221-U Facility (U-Plant).* PNNL-14908, Pacific Northwest National Laboratory, Richland, Washington.