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E-Area Low-Level Waste Facility GoldSim System Model

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EXECUTIVE SUMMARY

This report documents the development of the E-Area Low-Level Waste Facility (ELLWF) trench system model. The GoldSim® Monte Carlo simulation software (GTG, 2018) is utilized to model the release and transport of radiological inventory disposed (both currently and in the future) within Engineered and Slit Trenches. This model is in support of the sensitivity and uncertainty analysis for the ELLWF Performance Assessment. The ELLWF system model utilizes a hybrid-approach to accurately describe the disposal system. The Hydrologic Evaluation of Landfill Performance model provides the infiltration data to both PORFLOW (ACRi 2018) and GoldSim (GTG 2018). PORFLOW is used to calibrate the GoldSim model to ensure confidence in the stochastic results. Finally, the concentrations from GoldSim transport simulations are fed into the SRNL Dose Toolkit (Aleman 2019) to calculate dose impacts and assess plume interaction.

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LIST OF ABBREVIATIONS

CIG	Components-in-Grout
DU	Disposal Unit
ELLWF	E-Area Low-Level Waste Facility
ET	Engineered Trench
GSA	General Separations Areas
HELP	Hydrologic Evaluation of Landfill Performance
ILV	Intermediate Level (Waste) Vault
LAWV	Low Activity Waste Vault
LVZ	Lower Vadose Zone
NRCDA	Naval Reactor Component Disposal Area
PA	Performance Assessment
PO	Performance Objectives
POA	Point of Assessment
SAT	Saturated
SRNL	Savannah River National Laboratory
SRS	Savannah River Site
ST	Slit Trench
SUA	Sensitivity and Uncertainty Analysis
UVZ	Upper Vadose Zone
WZ	Waste Zone

1.0 Introduction

The GoldSim® Monte Carlo simulation software (GTG 2018) is utilized to model the release and transport of radiological inventory disposed (both currently and in the future) within Engineered and Slit Trenches. DOE Manual 435.1-1 stipulates that "The performance assessment shall include a sensitivity/uncertainty analysis." The General Separations Area (GSA) E-Area Low-Level Waste Facility (ELLWF) trench system model is part of the effort to address recommendations from the 2015 PA strategic planning team outlined by Butcher and Phifer (2016) to include sensitivity and uncertainty analysis (SUA) in the next revision of the ELLWF Performance Assessment (PA). SUA is necessary to provide a reasonable expectation that the performance objectives (PO) will be met.

The model can provide both deterministic and stochastic (probabilistic) results. The purpose of the GoldSim ELLWF trench system model is to generate a distribution of reasonable, potential dose exposures that an individual could experience via the groundwater exposure pathway. This probability distribution in dose exposure is a measure of the overall uncertainty arising from uncertainties embedded in the input parameters of the model. To capture the uncertainty, the "stochastic element" within GoldSim is utilized. This gives the user a means of explicitly accounting for the uncertainty associated with each input parameter. During probabilistic simulations, GoldSim applies the Monte Carlo technique across the set of stochastic elements within the model. The result of each probabilistic simulation is a distribution of uncertainty that represents the potential dose exposure. A review of each result is then compared against the POs, to determine if risk is managed properly.

Sensitivity analysis provides insight into the uncertainty inherent in the PA calculations and gives context to decision makers. One of the goals of sensitivity analysis is to identify which variables have distributions that exert the greatest influence on the variability of the dose. Stochastic parameters will have different sensitivities at different times because the major contributing radionuclide could be different. Quantitative assessment of the importance of inputs is necessary when the level of uncertainty in the concentration (and therefore dose) exceeds the acceptable threshold (or PO). Sensitivity and uncertainty results are useful in determining which parameters of the disposal facility should be the focus of future PA maintenance activities. These activities may include development of more rigorous analytical techniques, or enhanced efforts to more accurately quantify environmental, or other physical, parameters.

Interpretation of SUA is focused on performance of key safety functions of the engineered and natural features of the disposal facility that influence the magnitude and timing of the predicted peak dose. This is accomplished by identifying the structural, hydraulic, and chemical inputs and assumptions having a significant influence on the source term release from the disposal facility, flux to the water table and concentrations at the 100-m point of assessment (POA). The results of SUA simulations are used to identify features, events, and processes that are components of one or more key safety functions and can significantly influence the magnitude of the releases. From sensitivity analysis, the factors influencing timing can be understood as well as the effect of key assumptions.

The Savannah River Site (SRS) ELLWF consists of six types of disposal: Low Activity Waste Vault (LAWV), Intermediate Level Vault (ILV), Trenches [Slit Trenches (STs), Engineered Trenches (ETs), and Component-in-Grout (CIG) Trenches], and Naval Reactor Component Disposal Areas (NRCDAs). Only STs/ETs and NRCDAs are addressed in the GoldSim System Model. The remaining disposal units incorporate concrete barriers which are better represented by two-dimensional PORFLOW modeling. Thus, in the next PA, sensitivity analyses for the LAWV and ILV will be performed using PORFLOW modeling.

STs are below-grade earthen disposal units with vertical side slopes making them inaccessible by vehicle. Waste is typically deposited at the top on one end and pushed into the unit (bulk waste) or crane lifted into place (containerized waste). Each ST is generally laid out in a series of five narrow parallel trench rows. In the typical layout, each trench row is designed to be 20 feet deep, 20 feet wide, and 656 feet long with ten feet to 14 feet of undisturbed soil separating each parallel trench row. A set of five, 20-foot wide trench rows, are grouped together within a nominal 157-foot wide by 656-foot long disposal unit footprint forming a single ST.

ETs are also below grade earthen disposal units. ETs are vehicle-accessible with an open trench design spanning the entire width and length of the disposal unit footprint (nominal size, 656 feet long and 157 feet wide). To allow vehicle accessibility, trench sides are laid back with slopes ranging from 1.25:1 (horizontal:vertical) to 1.5:1. This design allows forklift and crane access to the interior of the trench for stacking of containerized waste primarily consisting of B-25 boxes and SeaLand containers.

Two at-grade gravel disposal pads are used as naval reactor component disposal areas, one within and the second adjacent to the ELLWF. These components arrive by rail and are moved by crane to at-grade gravel disposal pads. Naval reactor waste is comprised of highly radioactive reactor components consisting of activated corrosion-resistant metal alloy stored within thick carbon-steel casks, and auxiliary equipment contaminated on the surface with activated corrosion products at low levels and stored within thinner-walled bolted containers.

The 643-26E pad, currently operating, is located within the ELLWF. The corner coordinates of 643-26E have changed since the 2008 E-Area PA to make room for adjacent engineered trenches (ET03 and ET04) on two sides of the pad. Using the current coordinates, the total area of 643-26E is 4,430 m^2. The 643-7E NRCDA is located adjacent to the ELLWF and is 546 m^2. The 643-7E disposal pad is closed to future receipts. In 2004, soil was mounded around and over containers for shielding.

A description of the key design and operational features of ELLWF disposal units is found in several PA documents (Nichols 2020, Dyer 2019, Danielson 2019, Wohlwend and Butcher 2018).

2.0 Model Description

The overall structure and flow diagram of the system model is shown in Figure 2-1. The five main configuration-controlled PA data sources are used to standardize key inputs to all the models to ensure consistency throughout the PA calculations. Four separate sub-models comprise the overall “system” model: The Hydrologic Evaluation of Landfill Performance (HELP), PORFLOW, GoldSim, and the SRNL Dose ToolKit. The HELP model provides the infiltration data to both PORFLOW and GoldSim. PORFLOW generates the flow fields used by GoldSim and is used to calibrate the GoldSim model to ensure confidence in the stochastic results. Finally, the concentrations from GoldSim transport simulations are fed into the SRNL Dose Toolkit to calculate dose impacts. These model components and interfaces are described below.

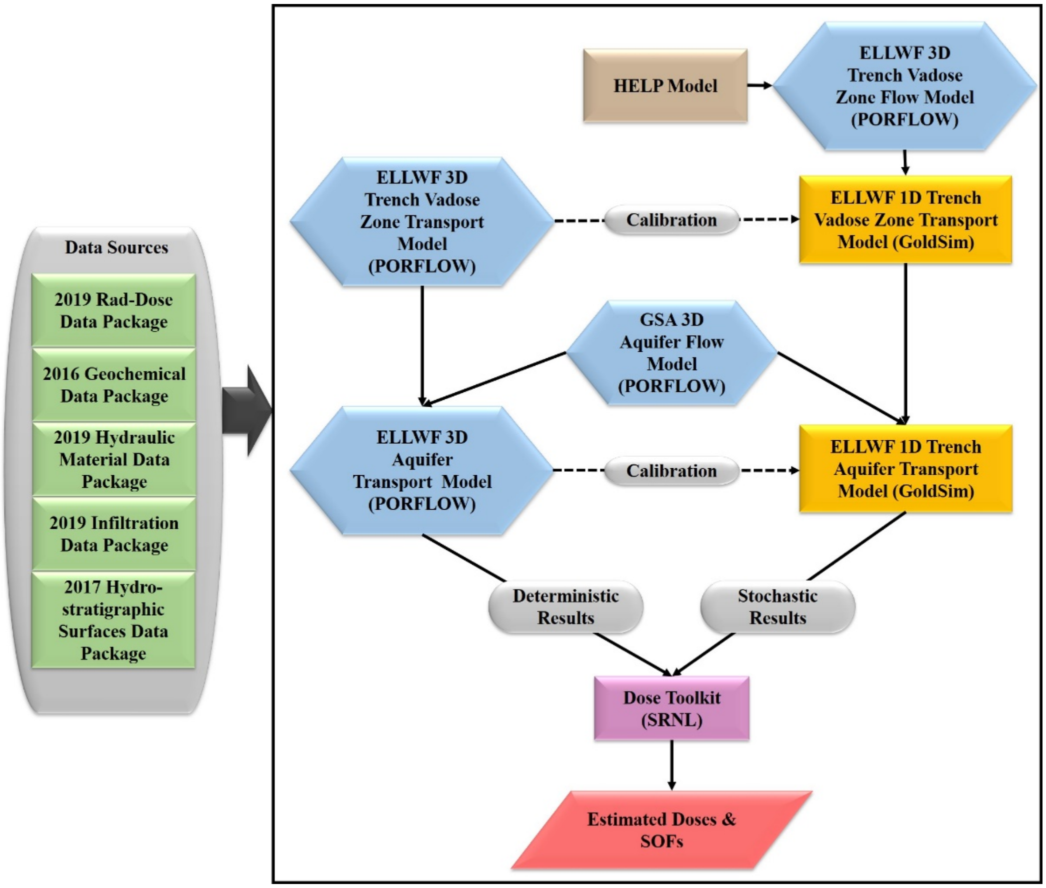

Figure 2-1. Flow diagram of system model.

2.1 Overview of Model Components and Interfaces

Data Sources. A significant amount of hydraulic properties data and hydro-stratigraphic information exists for the GSA, and several of the major facilities within the GSA have had PA or closure analyses performed in earlier years. Key input data sources are maintained within SRNL and are referred to as Data Packages (i.e., they are routinely updated as new approved data becomes available and are maintained under the E-Area PA maintenance program). As listed in Figure 2-1, the key data sources are the:

- **2019 Rad-Dose Data Package** – This data package (Smith et al. 2019) contains all the up-to-date radiological information for 1252 radionuclides (based on the ICRP Publication 107) including parameters such as half-life, decay modes, dose conversion factors for internal and external exposure, maximum contaminant levels, and human consumption factors;
- **2016 Geochemical Data Package** – This data package (Kaplan 2016) contains all the up-to-date geochemical information for the various materials typically considered in fate and transport analyses of SRS facilities including parameters such as sorption coefficients (K_d values), liquid-phase solubilities, and chemical leach factors;
- **2019 Hydraulic Properties Data Package** – This data package (Nichols 2020) contains up-to-date hydraulic property estimates for the soils, cementitious materials, and waste zones associated with the ELLWF engineered and natural disposal system including parameters such as porosity, dry bulk density, particle density, saturated hydraulic conductivity, characteristics curves and effective diffusion coefficients;

- **2019 Infiltration Data Package -** This data package (Dyer 2019) contains all the up-to-date information on the cap design and material properties assumptions, and the modeling results for the HELP infiltration model simulations performed to establish the upper boundary condition for the PORFLOW vadose-zone flow model for the various E-Area disposal unit types; and
- **2017 Hydro-stratigraphic Surfaces Data Package** – This data package (Bagwell and Bennett 2017) contains all the up-to-date estimates of ELLWF disposal units subsurface elevations and depths for the water table, lower aquifer zone, Upper Three Runs aquifer, Tan Clay confining zone, and Tobacco Road Sand zone.

All data are imported into the model as either GoldSim Data Elements or Time Series Elements. Data Elements are used to contain radionuclide data, and hydraulic and geochemical data organized by material type. Infiltration estimate tables are contained in Time Series Elements.

HELP Model. Infiltration modeling results from HELP model simulations were used to establish the upper boundary conditions for the PORFLOW vadose zone flow model for all E-Area disposal unit types (Dyer 2019).

For STs and ETs, infiltration estimates were produced for both intact and subsided case conditions. For worst-case subsidence scenarios, localized catastrophic failures of the closure cap are assumed for sections of closure cap underlain by “non-crushable” containers. These containers are assumed to simultaneously fail immediately upon installation of the final closure cap at the end of the 100-year institutional control period. Infiltration estimates through the closure cap are calculated based on the maximum areal extent occupied by non-crushable containers in the various STs and ETs.

HELP model infiltration estimates are produced for an intact-only cap simulation case for the NRCDA’s. Naval reactor components and auxiliary equipment are packaged in thick-walled welded casks and bolted steel containers which are assumed to not collapse until well after the end of the 1000-year post closure period.

Infiltration estimates for the various trench units and infiltration scenarios are provided in the Infiltration Data Package and utilized by the GoldSim model as described above under *Data Sources*.

PORFLOW Models. The recently updated PORFLOW-based 3D flow model, referred to as the GSA2018 flow model (Flach 2019), is being used to define the aquifer flow path for all the GoldSim disposal unit models. Although the GSA flow field could be used directly for PORFLOW aquifer transport simulations, SRNL has used flow information defined on a localized grid of smaller extent but higher resolution. To that end, a sub-region of the GSA2018 flow model underlying the ELLWF is subdivided into four refined “cutouts” for performing aquifer transport simulations in the next E-Area PA (Hang 2019). The flow field provided by these aquifer model cutouts is brought into GoldSim by providing an initial estimate of the aquifer Darcy velocity and geometric parameters.

PORFLOW transport results from detailed 3D vadose zone models and the 3D aquifer model are being used to support GoldSim calibration to PORFLOW deterministic results. Accounting for differences in infiltration boundary conditions, eighteen unique ST and ET vadose zone PORFLOW models, defined by seven hydro-stratigraphic groupings, will be used in the next E-Area PA (Danielson 2019). Disposal units were organized into these groupings based on similar depth to water table and clay thicknesses. A GoldSim trench model location will be selected and developed from five of the seven hydro-stratigraphic groupings along with a single NRCDA model to benchmark with the respective PORFLOW trench model at each location. Trench units and NRCDAs are considered “earthen” disposal units due to the absence of engineered barriers between the waste form and soil. The calibration utilizes PORFLOW fluxes to the water table and concentrations at the 100-m POA for the radionuclides being simulated.

PORFLOW deterministic analysis is also being used to quantify uncertainty in the release and transport of radionuclides from concrete disposal units, i.e., Low Activity Waste Vault and Intermediate Level Vault. These two approaches, deterministic PORFLOW analysis and probabilistic GoldSim analysis, form a hybrid approach to evaluating total disposal system uncertainty.

SRNL Dose Model. The SRNL Dose Model Toolkit (Aleman 2019) performs a series of calculations using six separate software codes. First, concentration time series output for each parent and short-chain progeny radionuclide at the 100-m POA boundary are taken from GoldSim and PORFLOW groundwater simulations and used as input to the Pre-Dose module takes which expands the short-chain radionuclide decay chain results to produce full decay chain results (using the assumption of secular equilibrium). These expanded files are input to the SRNL PreDose Maximum Concentration module to generate composite 'worst case' full-chain concentration history profiles for each existing/future inventory scenario for input to the SRNL PA/CA Limits and Doses Tool and compared to DOE 435.1 performance objectives and measures. The output of this tool is a series of concentration and dose files for each ground water pathway where contributions from each full chain progeny have been rolled up to the parent nuclide on a per Ci of parent buried basis and are used as input to the SRNL ELLWF Dose Investigation Tool. This tool is designed to quantify the dose impact to groundwater protection and all-pathways human dose receptors at the POA 100-meter boundary surrounding the ELLWF. This POA boundary comprises a 'curtain' of PORFLOW aquifer model computational cells where concentrations of select parent radionuclides and short-chain radioactive progeny are calculated and recorded at a specified time frequency. The total time history of the calculation encompasses the period-of-performance for groundwater protection and all-pathways.

For GoldSim simulations, the maximum concentration time series for each parent radionuclide and short-chain progeny at the 100-m POA are exported into an Excel workbook. The workbook is then transferred to the SRNL Dose Toolkit directory where it is read into the initial PreDose Module as a list-directed input file.

Full descriptions of these system model components are contained in the references provided in the above summaries. The final system model component, the GoldSim sub-model, is discussed in the next section.

2.2 GoldSim Sub-Models

The remainder of this report focuses on the GoldSim sub-models as illustrated in Figure 2-2. ELLWF Trench GoldSim Models are being built with the GoldSim version 12.1.3 #192 (March 13, 2019). Trench units representing five of the seven unique hydro-stratigraphic zones defined by Danielson (2019) along with one NRCDA have been selected as locations for GoldSim models as discussed in Section 2.2.6. These disposal units are ST06, ST10, ST17, ET02, ET08 (Plot 8 center unit), and NR26E (643-26E NRCDA). The following discussion is generally applicable to all the GoldSim models but is focused on the development of the first GoldSim model in the ST06 footprint.

Contaminant transport in the porous medium water phase includes the following advective processes: infiltration of precipitation from the ground surface, downward migration through the vadose zone, recharge (from the bottom of the vadose zone) of the aquifer at the water table, and lateral transport in the saturated zone to the 100-m POA. The ST06 model, currently under development, utilizes the PORFLOW ET geometry and waste properties in order to simplify the initial model calibration. Ultimately, both STs and ETs will be modeled and calibrated within the ELLWF GoldSim Model.

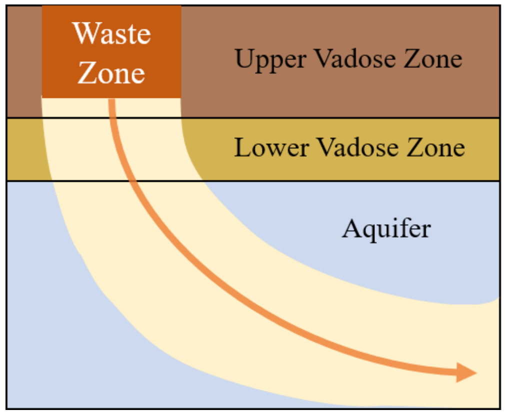

Figure 2-2. GoldSim ELLWF trench conceptual model.

2.2.1 Inventory

The inventory is uniformly distributed within the waste zone at the time operations begin in the trench. The inventory placed into the waste zone is controlled by dashboard buttons. For the system model, there are currently seven radionuclides of interest: I-129, H-3, C-14, Tc-99, Sr-90, U-238, and Np-237. The short chain progeny (one-year half-life cutoff value) of U-238 and Np-237 are also included in the inventory:

- U-238→U-234→Th-230→Ra-226→Pb-210
- Np-237→U-233→Th-229.

The species list contains 14 radionuclides, the seven parents and six daughters. Additional radionuclides may be added based on results of the ongoing radionuclide screening. All of the radionuclide inventory is treated as "generic" meaning it is immediately available for release at the time of emplacement (i.e., no credit for the container or waste form in radionuclide holdup). Through the dashboard, the user can choose to run the model with either a 1 Ci inventory or the projected inventory at closure.

2.2.2 Radionuclide and Material Properties

The "Material" container includes definitions of radionuclide contaminant species and their decay rates, and the bulk physical and hydraulic properties of the materials making up the solid porous media. The radionuclide data for the species modeled are obtained from the SRNL Radionuclide-Dose data package (Kaplan 2016) and given in Table 2-1. Radionuclide properties are well known and therefore not assigned uncertainty distributions.

Table 2-1. Radionuclide data for species modeled.

Species ID	Atomic Weight (g/mol)	Half-life (year)	Daughter
C-14	14	5.70E+03	
H-3	3	1.23E+01	
I-129	129	1.57E+07	
Np-237	237	2.14E+06	U-233
Pb-210	210	2.22E+01	
Ra-226	226	1.60E+03	Pb-210
Sr-90	90	2.88E+01	

Species ID	Atomic Weight (g/mol)	Half-life (year)	Daughter
Tc-99	99	2.11E+05	
Th-229	229	7.34E+03	
Th-230	230	7.54E+04	Ra-226
U-233	233	1.59E+05	Th-229
U-234	234	2.46E+05	Th-230
U-238	238	4.47E+09	U-234

The model represents five porous media zones comprising the disposal system including: the waste zone (WZ), upper vadose zone (UVZ), lower vadose zone (LVZ) and saturated (SAT) zone. The hydraulic properties within these zones employ the following six material types defined by Nichols (2020): ET Waste before dynamic compaction, ET waste after dynamic compaction, ClayeySoil (UVZ), SandySoil (LVZ), SatSandySoil, and SatClayeySoil.

Differences in bulk material properties between saturated and unsaturated zone soils are based on recommendations from the Hydraulic Properties Data Package for using effective material properties in the saturated zone (Nichols 2020). Effective saturated zone material properties have been assigned based on the knowledge that total porosity overestimates the effective porosity that participates in contaminant transport due to the presence of dead-end pore spaces and intermittent clay lenses.

Though ET waste zone properties are being assumed in ST06 for initial testing and calibration, ST waste properties will be used in the PA. ST waste zone properties are taken to be those of the "hybrid" ST defined in Phifer (2010). A "hybrid' ST waste zone representation was developed that combines bulk waste and containerized waste properties in a manner that conserves mass so that radionuclide retardation is not unduly conservative or non-conservative. Because a ST receives both bulk and containerized waste throughout a trench, a "hybrid" waste zone is assumed by combining the two waste types into a set of equivalent properties based on an estimated fraction of each waste type.

Properties of the porous media are defined in separate containers for each material type. Nominal parameter values for dry bulk density, porosity, and saturated effective diffusion coefficient for each material type are given in Table 2-2.

Table 2-2. System model material properties.

Material	Dry Bulk Density (g/cm3)	Porosity	Effective Diffusion Coefficient (cm^2/yr)
ET Waste Before Compaction	0.282*	0.893	1.67E+02
ET Waste After Compaction	1.81*	0.317	1.26E+02
ClayeySoil (UVZ)	1.65	0.385	1.67E+02
SandySoil (LVZ)	1.62	0.395	1.67E+02
SatSandySoil	1.04	0.250	1.67E+02
SatClayeySoil	1.04	0.250	1.26E+02

*Dry bulk density of waste is dependent on the particle density (2.65 g/cm3) and the porosity: Dry Bulk Density=Particle Density * (1 - Porosity)

Representation of hydraulic property value uncertainty for the E-Area vadose zone soils above are based on statistics on site-specific field and laboratory data or literature-based values as described in Nichols

(2020). Explicit uncertainty representation for the E-Area disposal unit waste zones is not provided due to the lack of data from which to derive such a representation.

Best estimate soil/water partition coefficients (K_ds) for the various solid materials are defined for each chemical element in the model (not each radionuclide species, e.g., a single K_d is assigned to all isotopes of uranium). ClayeySoil and SandySoil K_ds are assigned to radionuclides in the different material zones in the model (i.e., WZ, UVZ, LVZ, and SAT zone) based on the chemical characteristics of the material types as shown below:

- ClayeySoil K_ds – WZ, ClayeySoil, SatClayeySoil
- SandySoil K_ds – SandySoil, SatSandySoil

ClayeySoil K_ds are assigned to radionuclides in the WZ (i.e., waste cells in the model) as the geochemistry of ClayeySoil is assumed to approximate that of the rusted metal waste containers. Sorption coefficients are given in Table 2-3. In the current model, uncertainty distributions for these best estimate K_d values are derived from Kaplan (2016). All K_d values are normally distributed with a standard deviation of $0.5*K_d$ in saturated clayey and sandy soils (in the Sat. Zone), $0.125*K_d$ in sandy soils and $0.25*K_d$ in clayey soils. Additionally, the K_d range is from a minimum of $0.25*K_d$ to a maximum of $1.75*K_d$ for sandy soils and $0.5*K_d$ to $1.5*K_d$ for clayey soils, as recommended in Kaplan (2016).

Table 2-3. Mean Soil/Water partition coefficients.

Element	Best Sand K_d (mL/g)	Best Clay K_d (mL/g)
C	1.0E+00	3.0E+01
H	0.0E+00	0.0E+00
I	1.0E+00	3.0E+00
Np	3.0E+00	9.0E+00
Pb	2.0E+03	5.0E+03
Ra	2.5E+01	1.8E+02
Sr	5.0E+00	1.7E+01
Tc	6.0E-01	1.8E+00
Th	9.0E+02	2.0E+03
U	3.0E+02	4.0E+02

2.2.3 Flow Rate and Saturation

The closure cap is not explicitly modeled within the ELLWF Trench GoldSim Model, it is implicitly accounted for by utilizing modified flow rates and saturation values provided by the PORFLOW vadose zone flow model. In the ELLWF Trench GoldSim Model, infiltration refers to the rate of water flowing downward (only the vertical component) into the waste zone. Before the surface interim runoff cover is applied, infiltration through the operational soil cover is assumed to be 15.78 in/yr, the annual-average rainfall minus the annual average evapotranspiration and surface runoff (Dyer 2019). While the interim cover is in place (assumed to be a geomembrane) and before the final closure cap is applied, the infiltration rate is 0.1 in/yr. Infiltration through the final closure cap varies through time due to cap degradation and is predicted by HELP and given in Dyer (2019). In addition to the infiltration rate through the cap, the saturated hydraulic conductivity of the unsaturated media (waste and clayey/sandy layers that make up the vadose zone) are incorporated into the PORFLOW vadose zone flow model to provide flow rates and saturation values for each section of the unsaturated zone through time. These are incorporated into the ELLWF Trench GoldSim Model in the form of time-series elements. A description of two closure cap conditions, intact and subsided, and their impact on infiltration and flow fields is provided below.

2.2.3.1 Intact Case

The infiltration into the waste zone is impacted by the condition of the intact closure cap over time and has a graded impact on radionuclide transport. This intact case represents the condition where uniform subsidence of the waste zone and slow deterioration of closure cap barriers (ex. high-density polyethylene geomembrane layer) over time gradually degrade the "safety function" provided by the closure cap. The HELP infiltration model sensitivity studies (Dyer 2019) generated infiltration profiles over a 10,000-year period for most-optimistic, best-estimate, and most-pessimistic intact scenarios. The infiltration rate time history for each scenario is given in Table 2-4. Note that these values begin at year zero when the cap is installed; therefore, zero in Table 2-4 is year 171 in the simulation because cap placement is at year 2165 and the simulation begins at the start of ELLWF operations in year 1994.

Table 2-4. Infiltration rate profiles for intact closure cap.

	Infiltration Rate (inches/year)		
Time after Cap placed (year)	**Most Pessimistic**	**Best Estimate**	**Most Optimistic**
0	8.80E-04	1.80E-04	4.15E-05
100	3.92E-02	4.52E-03	2.50E-04
180	1.85E-01	2.89E-02	2.05E-03
290	6.42E-01	1.33E-01	1.26E-02
300	7.00E-01	1.48E-01	1.44E-02
340	9.58E-01	2.19E-01	2.33E-02
380	1.26E+00	3.11E-01	3.56E-02
560	2.99E+00	1.02E+00	1.57E-01
1000	7.30E+00	4.41E+00	1.30E+00
1800	1.05E+01	9.18E+00	6.09E+00
2623	1.13E+01	1.06E+01	9.02E+00
3200	1.15E+01	1.09E+01	9.80E+00
5600	1.17E+01	1.13E+01	1.05E+01
10000	1.18E+01	1.13E+01	1.06E+01

In addition to the three infiltration rate scenarios, there are two saturated hydraulic conductivity (Best Estimate and Conservative) cases for each material type (i.e.: two for clayey soils and two for sandy soils) present in the unsaturated zone as well. Each combination of infiltration rate and saturated hydraulic conductivity case produces a unique PORFLOW vadose zone flow field (12 in total). The PORFLOW-generated flow fields provide spatially averaged velocities and saturation values that are used as input to the GoldSim model in the form of time-series elements. To address uncertainty and sensitivity, the GoldSim model randomly samples from the set of 12 possible combinations.

2.2.3.2 Subsided Cases

Subsided cases, as distinct from the intact case described above, are the result of localized waste zone failures that create subsidence areas (or holes) in the overlying closure cap surface. These localized failures are caused by containers and equipment that are assumed to not collapse during previous waste stabilization measures, such as dynamic compaction, but instead fail catastrophically immediately upon installation of the final multilayer closure cap. This category of containers is described as "non-crushable". The area under the subsidence region is modeled in parallel with the intact region. While the infiltration through the intact region is directly obtained by HELP (Dyer 2019), the infiltration through a subsided region (hole) is dependent on the hole size and location with respect to the crest of the closure cap as shown schematically in Figure 2-3. Increased infiltration due to subsidence is the result of runoff into the hole from the upslope intact portion of the cap and lateral drainage layer. Where subsided infiltration, I_S, is estimated by the equation shown in Figure 2-3, where I_B is the background infiltration (16.5 in/yr; the annual-average rainfall minus the annual average evapotranspiration), L_H is the length of the hole (100 ft based on 2% subsidence from Danielson (2019)), I_I is the intact infiltration rate (Table 2-4), L_U is the length of the intact upslope area that is dependent on the hole location. The location of the hole is controlled by a dashboard input element where the range of hole positions is described by:

0: Hole location controlled by discrete distribution (End, Middle, and Crest have the same probability)
1: End (single hole in cap at end of trench with highest infiltration)
2: Middle (single hole midway between crest of cap and end of trench)
3: Crest (single hole at crest of cap with lowest hole infiltration)

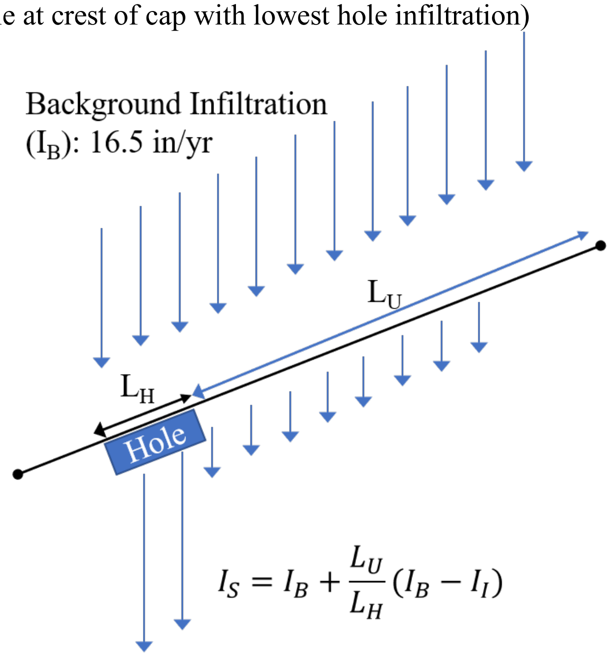

Figure 2-3. Schematic of subsided infiltration.

During stochastic simulations, the hole choice will be "0" as that will allow the hole location to be sampled randomly for each realization. Similar to the intact flow rate methodology, each hole location provides a unique infiltration rate at the subsided region and will produce coupled flow rates and saturation values that will be utilized as input to the GoldSim model in the form of flow rate and soil saturation time-series elements for each layer in the unsaturated zone (WZ, UVZ, LVZ).

2.2.4 Chronology

During the operational period, low-level waste is typically disposed within the trenches beginning at one end of the trench unit and proceeding toward the other end. In the system model, however, an entire ST is assumed to be filled immediately upon receipt of the first waste package in any particular waste unit. Trench closure is then conducted in stages. Operational closure consists of a minimum 4-foot thick clean soil layer placed over the waste (i.e., operational soil cover) sloped for positive drainage away from the trench. For STs, this is followed by installation of a surface geomembrane runoff cover (i.e., operational runoff cover) assumed to occur no later than four years following the trench being filled with waste. These covers are assumed to be maintained (i.e., no change in infiltration) until the end of the operational period for E-Area, at which time these operational runoff covers are either replaced or, if still serviceable, simply incorporated into an area-wide geomembrane cover over all closed trench units (i.e., interim closure). For ETs, a geomembrane cover is not installed until 2040 or the start of institutional control in 2065 depending on when an ET is operational. This interim cover is assumed to be maintained throughout the 100-year institutional control period. Final closure by a multi-layer, soil-geomembrane closure cap over all disposal units (i.e., ST's, ET's, ILV, LAWV, NRCDA's) will take place at the end of the assumed 100-year institutional control period. Performance is assessed throughout the operational and institutional control periods and beyond over a 1,000-yr post-closure period.

Within the model, the GoldSim "Chronology" container defines all model events. The condition and status of the site during any period are controlled by data elements based on actual and projected disposal unit (DU) lifecycles. These data elements are then utilized to create milestones and status elements based on when (in model time) these events occur. Waste emplacement occurs when the "Open_ST" status element is triggered by the "OpsOpened_ST" milestone. Similarly, the estimated infiltration rate into the waste zone is modified by the status elements "Cap_None", "Cap_Operational", and "Cap_Final" which are functions of "OpsOpened_ST," "OpsClosed_ST," and "ClosureCap_Constructed" milestones, respectively. Subsidence is triggered by the "ClosureCap_Constructed" milestone. This is graphically shown in Figure 2-4 where the dates are specific to ST06.

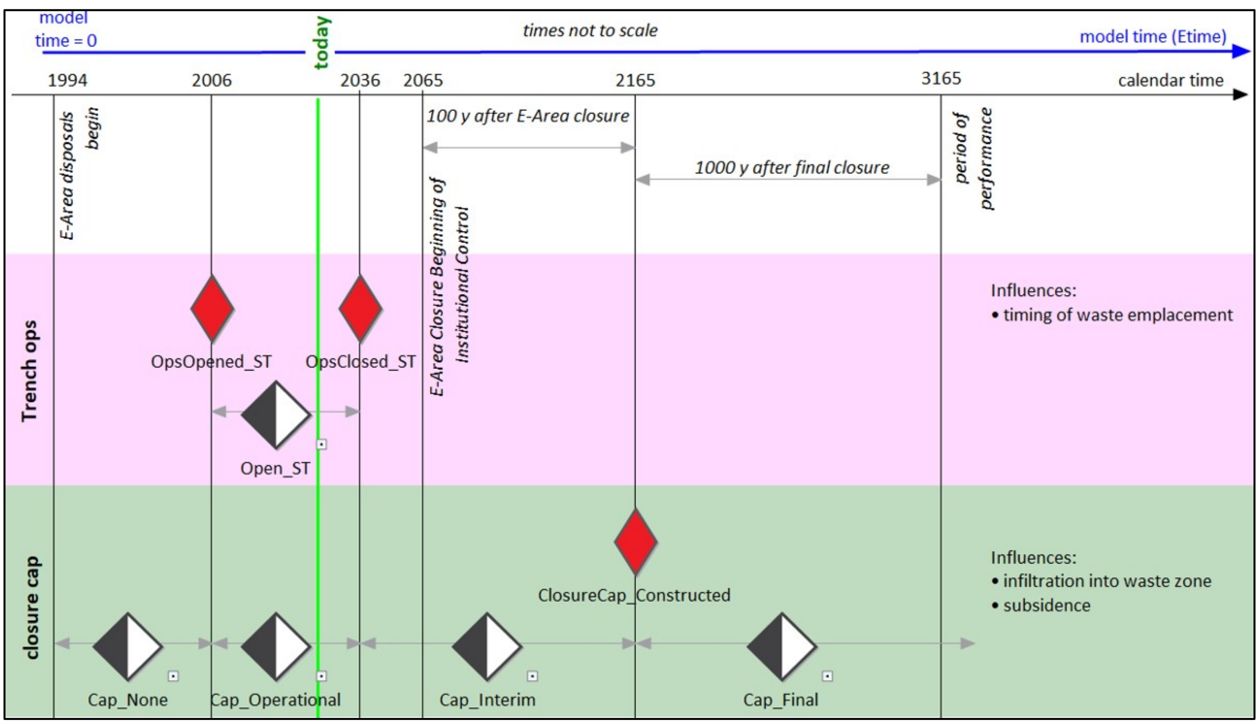

Figure 2-4. System model chronology for ST06.

Infiltration begins when the entire inventory is placed within the waste zone on the date each trench becomes operational ("OpsOpened_ST"). This initial infiltration following waste emplacement is through the operational soil cover until the operational runoff (plastic geomembrane) cover is installed ("OpsClosed_ST"). The infiltration then changes to the Interim infiltration (i.e., a greatly reduced infiltration rate through the relatively impermeable geomembrane). This infiltration rate is maintained until the end of the 100-year institutional control period when the final closure cap is installed. Subsidence is assumed to occur immediately after the final cap is placed in 2165 (100 years after the assumed E-Area closure date of 2065) as described in Section 2.2.3.2, followed by gradual closure cap degradation resulting in changes to infiltration throughout the post-closure period as described in Section 2.2.3.1. Peak impacts for highly-sorbed radionuclides may occur after 1,000 years for near-surface disposal facilities. To address the potential peaks in the far future, sensitivity and uncertainty analysis calculations can be extended for several thousand more years.

2.2.5 Stochastic Parameters

Uncertainty analysis is concerned with how the uncertainty in stochastic model input parameters is propagated through the model to the selected model results. Sensitivity analysis is focused on determining which of the many input parameters are most influential in contributing to the overall uncertainty in the model. Stochastic elements are intended to capture the overall parameter uncertainty in the model. These do not address conceptual model uncertainty or that induced by model structure, such as discretization.

It is important to establish and understand potential sources of uncertainty and biases in the model so that conclusions drawn in these studies account for the stochastic behavior of the system and predictions of long-term performance are reasonably accurate. Uncertainty in models can arise from multiple sources including parametric uncertainty, which is caused by the lack of knowledge of the exact values that model parameters should take in the simulations. There is a need to examine the sensitivity of model predictions to uncertainties in input parameters. A comprehensive SUA should help to identify important physical processes affecting outcome and determine what model components explain most of the model uncertainty. Those parameters that are not well known or poorly characterized were selected for variable input if judged to have a significant effect on the calculated groundwater concentrations and dose, as determined by previous sensitivity analyses, or professional judgment. The Monte Carlo analysis performed by the GoldSim program generates a statistical distribution of groundwater concentration propagated from these uncertain input parameters. Groundwater concentrations are then fed into the SRNL Dose Toolkit to generate a statistical distribution of dose impacts.

Sensitivity analysis is limited by the uncertainty assigned to input parameters. For some parameters, uncertainty is well defined based on statistics calculated for a set of sample results (e.g., E-Area soil physical properties properties). For other input parameters, a stochastic distribution of values is not as well-known and are assigned based on a data review (e.g., chemical sorption or K_d's). In cases with little or no data available, a pre-determined range of uncertainty behavior (e.g., triangular, uniform or discrete distribution of uncertainty) is assigned based on different levels of optimism/pessimism (e.g., infiltration). Using these pre-determined uncertainty distributions provides insight on the importance of these type parameters to overall performance. The remaining input parameters in the model were not defined by stochastic elements for a variety of reasons. Some deterministic inputs are well characterized (e.g., radionuclide half-lives), others are assigned reasonably bounding (conservative) values, and, finally, some are to be treated outside of the SUA framework (e.g., inventory uncertainty to be examined as part of the closure analysis through scaling of the deterministic results). The stochastic elements within the System Model are listed in Table 2-5.

Table 2-5. List of Stochastic Elements in the ELLWF Trench GoldSim Model

Stochastic Element Name	Description
Infiltration	Discrete distribution of equally weighted infiltration cases
Waste_HydraulicCond	Discrete distribution of equally weighted waste saturated hydraulic conductivity cases
Clayey_HydraulicCond	Discrete distribution of equally weighted clayey soil saturated hydraulic conductivity cases
Sandy_HydraulicCond	Discrete distribution of equally weighted sandy soil saturated hydraulic conductivity cases
Hole_Location_Stoch	Samples the choice of hole location
SatZoneDarcyVel_byUnit	Samples the saturated zone Darcy velocity by disposal unit
NonCrushWasteDist	Samples the percent waste that is non-crushable
DryBulkDensity_ClayeySoil	Samples the clayey soil dry bulk density
DryBulkDensity_SandySoil	Samples the sandy soil dry bulk density
Porosity_ClayeySoil	Samples the clayey soil porosity
Porosity_SandySoil	Samples the sandy soil porosity
Kd_Dist (Clayey Soil)	Samples uncertainty in the K_d values for transport through clayey soil; waste assumes this distribution as well
Kd_Dist (Sandy Soil)	Samples uncertainty in the K_d values for transport through sandy soil
FinalWasteThickness_ST	Samples the thickness of the waste layer after compaction
Depth_WT_stoch	Samples the uncertainty in the depth to the water table
Clay_thickness_stoch	Samples the uncertainty in the clayey thickness within the vadose zone
SatThickness_Stoch	Samples the uncertainty in the thickness of the saturated zone

2.2.6 Vadose Zone

The conceptual model of the vadose zone is shown schematically in Figure 2-5. The closure cap is not explicitly modeled but accounted by utilizing modified flow rates and saturation values provided by the PORFLOW vadose zone model. The vadose zone is modeled by two separate series of one-dimensional (1-D) Cell and Aquifer pathways. The two series represent areas within the trench that contain either crushable containers (intact cap case) or non-crushable containers (subsided cap case) as described in Section 2.2.3**.**.

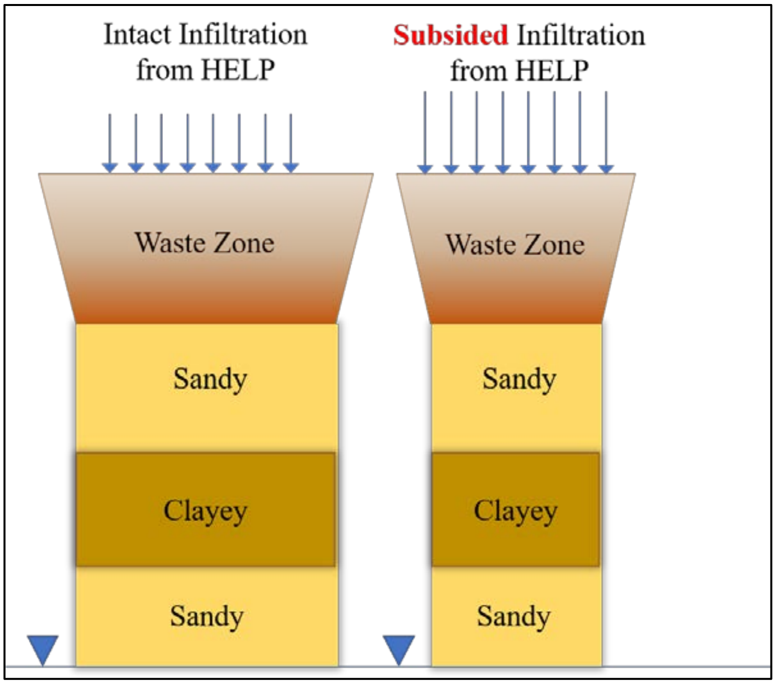

Figure 2-5. Schematic of the GoldSim vadose zone conceptual model

The waste zone is represented by a series of 1-D Cell pathways. The flow area is the product of the trench width (157 ft) and the length (656 ft). The area is also multiplied by the fraction of the waste that is either crushable or non-crushable depending which series the cells represent. To model dynamic compaction, the waste zone is separated into two sections: upper waste zone and lower waste zone as shown in Figure 2-6. The amount of inventory initially placed within each cell is based on the fraction of trench thickness it represents as shown in Eq. 1-1.

$$I_{Cell\_Upper} = I_{Total} * Frac_{Crushed} * \frac{Thickness_{Cell\_Upper}}{Thickness_{Total}}. \qquad \text{Eq. 1-1}$$

Where I_{Cell_Upper} is the inventory placed in each upper waste zone cell, I_{Total} is the total of inventory in the trench, $Frac_{Crushed}$ is the fraction of the trench that contains crushable waste, $Thickness_{Cell\_Upper}$ is the thickness of each upper waste zone cell, and $Thickness_{Total}$ is the total waste thickness. The inventory placed in each lower waste zone cells is analogous to that placed in the upper waste zone using the lower waste zone cell thickness. When the final cap is emplaced, the radionuclide inventory within the upper waste zone is transferred to the lower waste zone using a series of discrete change elements as well as a mass collector cell.

To be consistent with the PORFLOW vadose zone model, the flux then leaves the waste zone and enters the first sandy portion of the vadose zone. This section is modeled by a series of 1-D Cell pathways. After leaving the first sandy layer, it goes through first a clayey layer and then a final sandy layer, which are also modeled by a series of 1-D Cell pathways. Although many DUs have two layers of clayey soil separated by sandy layers, the clayey layers are combined in the system model. This is consistent with the PORFLOW vadose zone model and produces only a ~1% difference in flux to the water table. The representation of the vadose zone is given in Figure 2-7.

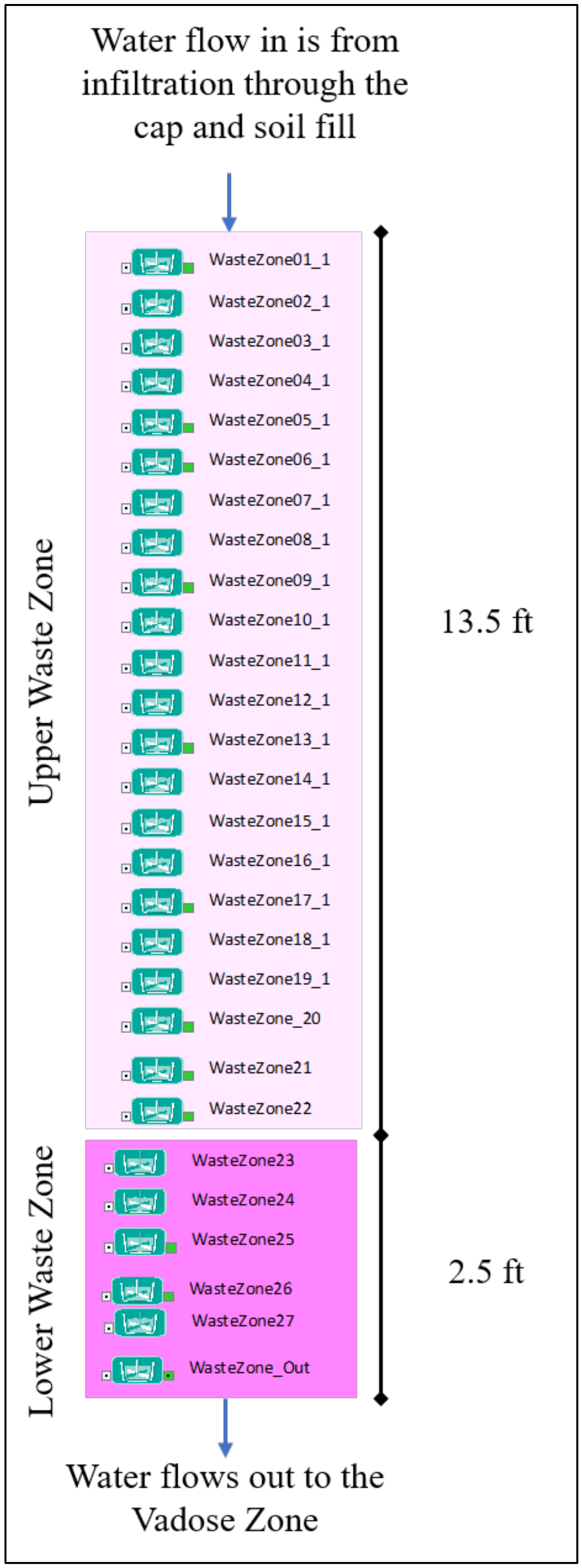

Figure 2-6. Representation of the waste zone.

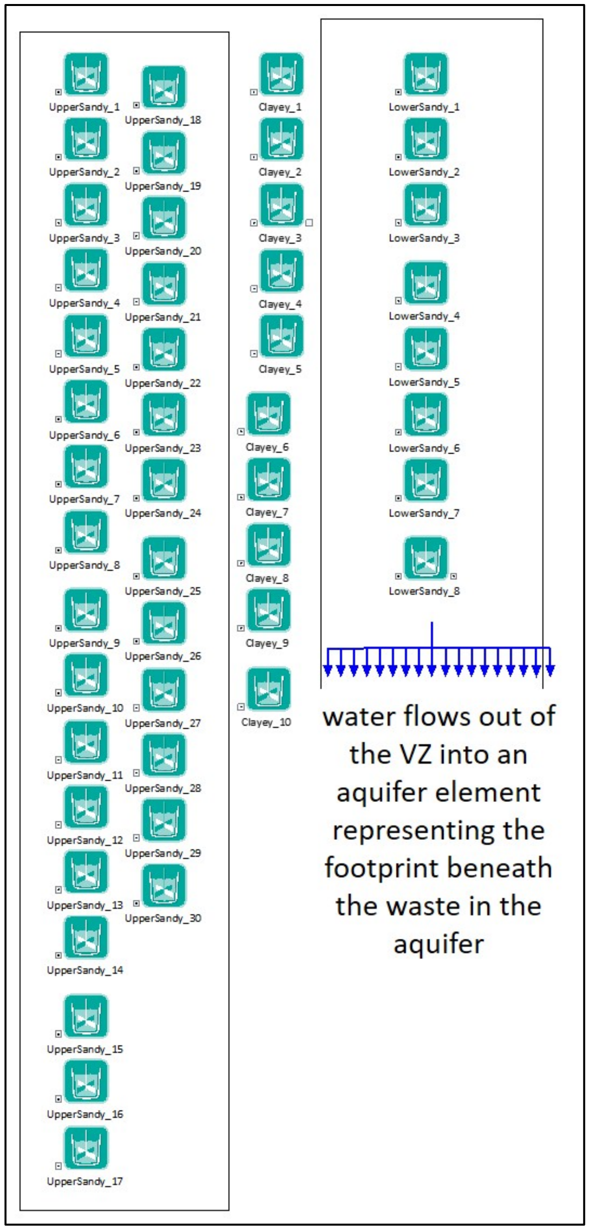

Figure 2-7. Representation of the vadose zone.

The flow area of the clayey and sandy sections is the same as that of the waste zone. The thickness of each material zone used in deterministic calculations assumes the minimum depth to the water table and the minimum clay thickness of each trench grouping as defined in Danielson (2019). The planned placement of trench units will span the entire E-Area footprint. The range of depths to the water table and clay layer thicknesses beneath trenches required use of multiple models to adequately represent hydro-stratigraphic features while maintaining a reasonable level of conservatism. In order to reduce the number of trench models analyzed in the PA, trench units were collected into seven hydro-stratigraphic groupings and a minimum clay thickness and depth to water table were selected as representative of each grouping. Trench units representing five of the seven unique hydro-stratigraphic zones defined by Danielson (2019) along with one NRCDA have been selected as locations for GoldSim models. The remaining two zones are considered to be adequately represented or bounded by the other five based on a comparison of relative depths to water table and clay thicknesses. The selected disposal units for the GoldSim models are ST06, ST10, ST17, ET02, ET08 (Plot 8 center unit), and NR26E (643-26E NRCDA). The depth to the water table and clay thickness statistics for each hydro-stratigraphic group are listed in Table 2-6 where the bold "Min" values are used for deterministic calculations.

Table 2-6. Depth to the water table and clay thickness statistics.

			Depth to Water Table (ft)				Clay Thickness (ft)			
Group ID	DU	DU #	**Min**	SD	Mean	Max	**Min**	SD	Mean	Max
1	ST08	8	**75.180**	0.925	76.347	78.051	**11.200**	1.125	12.444	14.187
1	ST09	9	**75.180**	0.925	76.347	78.051	**11.200**	1.125	12.444	14.187
1	ST10	10	**75.180**	0.925	76.347	78.051	**11.200**	1.125	12.444	14.187
1	ST11	11	**75.180**	0.925	76.347	78.051	**11.200**	1.125	12.444	14.187
1	ET04	24	**75.180**	0.925	76.347	78.051	**11.200**	1.125	12.444	14.187
1	ST01	1	**75.180**	0.925	76.347	78.051	**11.200**	1.125	12.444	14.187
1	ST02	2	**75.180**	0.925	76.347	78.051	**11.200**	1.125	12.444	14.187
2	ST03	3	**64.310**	3.410	69.496	72.932	**4.090**	1.400	6.155	7.705
2	ET03	23	**64.310**	3.410	69.496	72.932	**4.090**	1.400	6.155	7.705
2	ST04	4	**64.310**	3.410	69.496	72.932	**4.090**	1.400	6.155	7.705
2	ST23	19	**64.310**	3.410	69.496	72.932	**4.090**	1.400	6.155	7.705
3	ST24	20	**55.460**	2.103	58.644	61.139	**1.880**	0.500	2.376	3.078
3	ST05	5	**55.460**	2.103	58.644	61.139	**1.880**	0.500	2.376	3.078
3	ST06	6	**55.460**	2.103	58.644	61.139	**1.880**	0.500	2.376	3.078
3	ST07	7	**55.460**	2.103	58.644	61.139	**1.880**	0.500	2.376	3.078
4	ET01	21	**55.040**	1.301	56.336	57.637	**15.460**	0.648	16.110	16.758
4	ST14	12	**55.040**	1.301	56.336	57.637	**15.460**	0.648	16.110	16.758
5	ET05	25	**46.120**	1.305	48.971	50.799	**10.190**	1.102	12.178	13.345
5	ET06	26	**46.120**	1.305	48.971	50.799	**10.190**	1.102	12.178	13.345
5	ST17	13	**46.120**	1.305	48.971	50.799	**10.190**	1.102	12.178	13.345
5	ST18	14	**46.120**	1.305	48.971	50.799	**10.190**	1.102	12.178	13.345
5	ST19	15	**46.120**	1.305	48.971	50.799	**10.190**	1.102	12.178	13.345
5	ST20	16	**46.120**	1.305	48.971	50.799	**10.190**	1.102	12.178	13.345
5	ST21	17	**46.120**	1.305	48.971	50.799	**10.190**	1.102	12.178	13.345
5	ST22	18	**46.120**	1.305	48.971	50.799	**10.190**	1.102	12.178	13.345
6	ET02	22	**36.623**	11.769	47.870	62.794	**0.000**	7.313	5.891	16.610
7	ET07	27	**63.150**	3.033	63.148	65.380	**5.340**	0.318	5.339	5.789
7	ET08	28	**63.150**	3.033	63.148	65.380	**5.340**	0.318	5.339	5.789
7	ET09	29	**63.150**	3.033	63.148	65.380	**5.340**	0.318	5.339	5.789

Saturation in the vadose zone varies as a function of time and location because of cap degradation and subsequent increase in infiltration, and is estimated from PORFLOW modeling (Figure 2-8). In the GoldSim system model these are represented by time series elements.

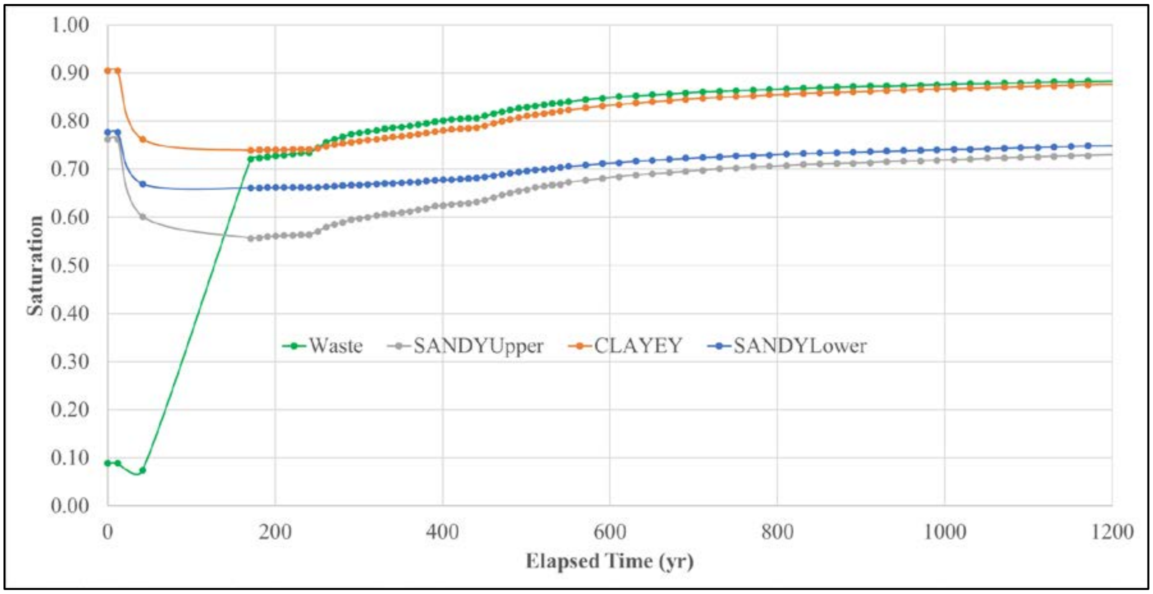

Figure 2-8. Saturation over time for each material in the vadose zone.

2.2.7 Aquifer

After transport through the vadose zone, the radionuclides enter the aquifer. Flux of contaminants from the vadose zone is transferred to an aquifer element that represents the footprint below the vadose zone. Multiple aquifer elements are then utilized to model the transport through the aquifer, ending at the 100-m POA. PORFLOW streamtraces emanating from the centers of each DU will be analyzed for travel distance and time to the 100-meter POA which will provide the length of the aquifer pathway and Darcy velocity for the GoldSim model. The initial estimate for Darcy velocity is the ratio of the PORFLOW travel distance and arrival time, times effective porosity (0.25). The aquifer thickness and width are estimated from concentration profiles of PORFLOW transport simulations using a steady-state source.

Because GoldSim models 1-D flow, the concentration of each aquifer element outflow represents the average concentration and 3-D spatial variation is not represented. This is conceptually different from the PORFLOW 3-D aquifer model that accounts for spatial variation and reports the maximum concentration at each POA. To be consistent with the PORFLOW transport simulations, plume function and plume multiplier factors are applied to each of the POA concentrations.

The plume function has eleven input arguments that account for the spatial variation (Tauxe, 2014) and produces a multiplier that varies between zero and one. The plume multiplier is a peaking factor that represents using the maximum concentration as opposed to the average concentration at each POA. The eleven arguments and their initial assigned values used in the plume function are given in Table 2-7. Figure 2-9 is a schematic that illustrates the physical meaning of many of the arguments. These values as well as the peaking factor will be varied during calibration.

Table 2-7. Plume function arguments.

Arguments	Description
X_L	Pathway length [1]
A	Cross-sectional area of the aquifer
L_s	Length of the source parallel to the flow direction [2]
X_V	Vertical position of the observation point [3]

Arguments	Description
X_T	Transverse position of the observation point [4]
D_s	Vertical depth to the top of the source from the top of the aquifer [5]
W_s	Width of the source, transverse to the aquifer flow [6]
b_s	Thickness of the source [7]
b	Thickness of the aquifer [8]
α_T	Dispersivity in the transverse direction
α_V	Dispersivity in the vertical direction

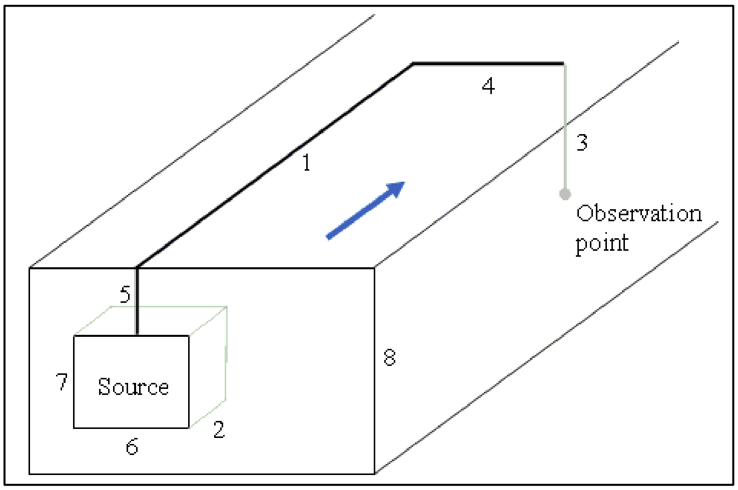

Figure 2-9. Schematic representation of the plume function.

2.2.8 Layout and Structure

The GoldSim ELLWF trench system model is comprised of multiple containers, Figure 2-10 shows containers that make up the system model. An overview of the layout and structure of the model is given below where container names are enclosed in quotes.

- "Material" contains the definitions of contaminant species and their decay rates, and the material properties of the physical materials making up the solid porous medias, and the fluid media, *Water*.
- "Inventory" includes definitions of the radionuclide inventory for the disposal units.
- "Simulation Settings" define the simulation controls and have two sub-containers:
    - "Chronology" defines the conditions and status of the site
        - "SlitTrench_Events" includes the timing of operational start/end, interim closure, and final closure
    - "Switches" includes multiple switches that can be used to control the behavior of the model and investigate the effects of model assumptions; many of these are controlled through dashboard controls
- "PhysicalProcesses" defines processes influencing contaminant transport
    - "WaterTransport_Vadose" includes data elements that describe water advection in the unsaturated (vadose) zone
        - "ClosureCap" contains the intact infiltration calculations (described in Section 2.2.3.1)
    - "WaterTransport_Aquifer" includes data elements that describe water advection in the saturated (aquifer) zone
    - "Subsidence" describes dynamic compaction as well as the parameters that define subsided infiltration (described in Section 2.2.3.2)

- "Documentation" provides useful illustrations describing the saturated zone and the plume function
- "Dashboards" stores the dashboards in the model; in general, all the dashboards are navigable from others, with the principal connection point in the Home dashboard
- "EngineeredSystems_Geometry" includes parameters for dimensions of the disposal units including area, length, and width as well as the thickness of the waste zone before and after compaction
- "NaturalSystems_Geometry" define parameters for dimensions, rates, and such for the natural materials surrounding the waste disposal units including:
    - Clayey layer thickness
    - Sandy layer thickness
    - Depth to water table
    - Aquifer thickness (thickness of Saturated Zone)
    - Aquifer width (width of Saturated Zone)
    - Distance to Seep
    - Distance to well comprised of clay
    - Distance to well comprised of sand
    - Well offset
    - Distance from well to seep
- "Miscellaneous" has elements defining Element Ones, Large, Ones and Small
- "Transport" includes the containers that hold the trench groundwater transport components, a snapshot of the container is shown in Figure 2-11
    - "WasteZone" contains two containers that hold the elements that model transport through the waste zone, one associated with the fraction of waste that is crushable at the end of IC and the other associated with the fraction of waste that is non-crushable at the end of IC
        - "WasteZone_Crushed" includes the elements used to define the geometry of the waste cells and the cell pathway elements that simulate the flow and transport of the inventory through the waste zone for waste that is considered crushable (described in Section 2.2.6)
        - "WasteZone_Noncrushed" includes the elements used to define the geometry of the waste cells and the cell pathway elements that simulate the flow and transport of the inventory through the waste zone for waste that is considered non-crushable (described in Section 2.2.6)
    - "VadoseZone" includes two containers that hold the elements that model transport through the vadose zone, one associated with the fraction of waste that is crushable at the end of IC and the other associated with the fraction of waste that is non-crushable at the end of IC
        - "VadoseZone_Crushed" includes the elements used to define the geometry of the vadose zone cells and the cell pathway elements that simulate the flow and transport of the inventory through the vadose zone for waste that is considered crushable (described in Section 2.2.6)
        - "VadoseZone_Noncrushed" includes the elements used to define the geometry of the vadose zone cells and the cell pathway elements that simulate the flow and transport of the inventory through the vadose zone for waste that is considered non-crushable (described in Section 2.2.6)
    - "WasteFootprint" includes the elements used to define the geometry of the footprint cells and the cell pathway elements that simulate the flow into each cell under the waste footprint from the unsaturated zone (described in Section 2.2.7)
    - "NearWell" includes the elements used to simulate flow and transport from the edge of the building to the 100-m well and elements used to define the plume function (described in Section 2.2.7)

- o "ToSeep" includes the elements used to simulate flow and transport from the 100-m well to the seep, as well as elements used to define the plume function (described in Section 2.2.7)

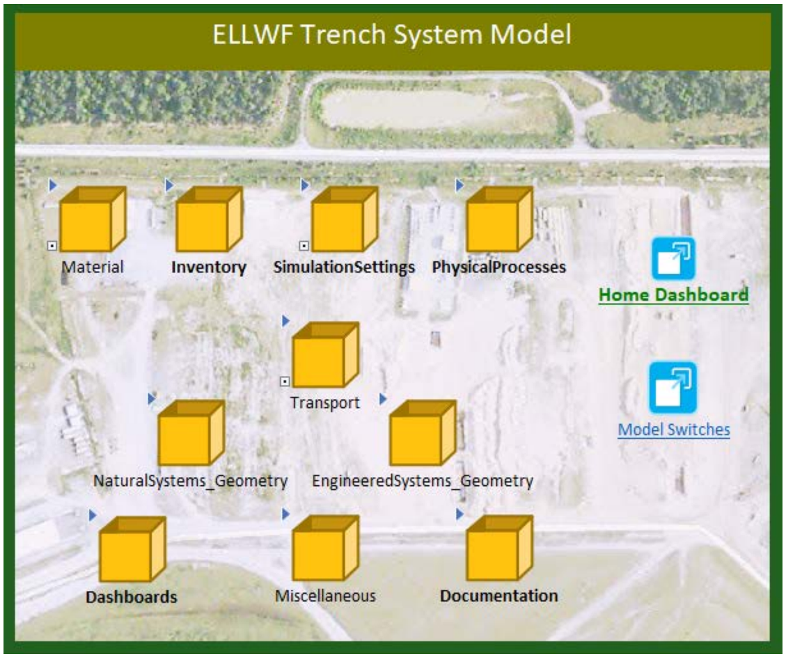

Figure 2-10. GoldSim ELLWF Trench System Model Home Screen.

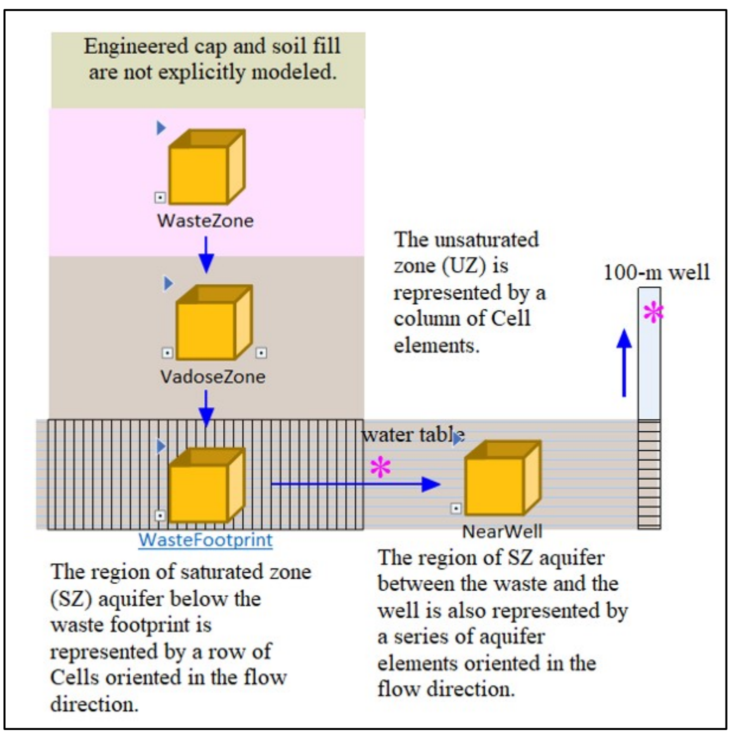

Figure 2-11. Transport Container Screen.

3.0 Conclusions

This report documents the development of the ELLWF trench system model. The various components of the total disposal system (closure cap, waste zone, vadose zone, aquifer and receptor exposure) are represented in different sub-models described in this report. A probabilistic approach using GoldSim® Monte Carlo simulation software (GTG 2018) is being employed to quantify uncertainty in the release and transport of radionuclides from earthen disposal units, i.e., Engineered Trenches, Slit Trenches and a Naval Reactor Component Disposal Area. This probabilistic approach is being combined with deterministic modeling using PORFLOW (ACRI 2018) to quantify uncertainty in the release and transport of radionuclides from concrete disposal units, i.e., Low Activity Waste Vault and Intermediate Level Vault. This hybrid-approach is intended to capture total disposal system uncertainty. The HELP model provides the infiltration data to PORFLOW and the resultant PORFLOW flow rate and saturation time-histories are imported into the GoldSim model. PORFLOW is then used to calibrate the GoldSim model to ensure confidence in the stochastic results. Finally, the concentrations from GoldSim transport simulations are used in the SRNL Dose Toolkit (Aleman 2019) to calculate dose impacts and assess plume interaction.

4.0 Future Work

Model development and calibration (vadose zone and aquifer) of the selected GoldSim trench model locations and the currently operating NRCDA is ongoing. PORFLOW is a higher-fidelity simulation of multi-dimensional transport phenomena while GoldSim is a 1-D transport model with a much lower computational time. Therefore, calibration to PORFLOW results is necessary to obtain accurate abstractions and to quantify the GoldSim model systemic bias resulting from reduced dimensionality.

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