Contract No:

This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-08SR22470 with the U.S. Department of Energy (DOE) Office of Environmental Management (EM).

We put science to work.™

Savannah River National Laboratory®

OPERATED BY SAVANNAH RIVER NUCLEAR SOLUTIONS

A U.S. DEPARTMENT OF ENERGY NATIONAL LABORATORY • SAVANNAH RIVER SITE • AIKEN, SC

GoldSim E-Area Low-Level Waste Facility Aquifer Zone Model Calibration Methodology

J. L. Wohlwend

L. L. Hamm

October 2020

SRNL-STI-2020-00346, Revision 0

SRNL.DOE.GOV

DISCLAIMER

Printed in the United States of America

Prepared for
U.S. Department of Energy

Keywords: *Sensitivity and Uncertainty Analysis, Monte Carlo, Modeling, PORFLOW*

Retention: *Permanent*

GoldSim E-Area Low-Level Waste Facility Aquifer Zone Model Calibration Methodology

J. L. Wohlwend
L. L. Hamm

October 2020

Prepared for the U.S. Department of Energy under contract number DE-AC09-08SR22470.

Savannah River National Laboratory®
OPERATED BY SAVANNAH RIVER NUCLEAR SOLUTIONS

REVIEWS AND APPROVALS

AUTHORS:

____

J. L. Wohlwend, Environmental Sciences & Dosimetry, SRNL Date

____

L. L. Hamm, Advanced Modeling, Simulation, and Analytics, SRNL Date

TECHNICAL REVIEW:

____

B. T. Butcher, Environmental and Biological Sciences, SRNL Date

APPROVAL:

____

D. G. Jackson, Manager Environmental Sciences & Dosimetry, SRNL Date

____

P. L. Lee, Manager Advanced Modeling, Simulation, and Analytics, SRNL Date

____

B. D. Lee, Director Environmental and Biological Sciences, SRNL Date

EXECUTIVE SUMMARY

This report documents the development and calibration of the E-Area Low-Level Waste Facility (ELLWF) GoldSim aquifer model. It provides a methodology on how a GoldSim aquifer model can be calibrated to specific PORFLOW-based aquifer predictions. The calibration activity presented within this report focuses on the Slit Trench #06 (ST06) location that resides within the center set of Slit Trenches. This GoldSim-based aquifer model is a generic model capable of being calibrated to any of the other trench locations within E-Area. In addition, subsequent activities (beyond the scope of this effort) will couple this GoldSim-based aquifer model to various GoldSim-based trench models, with the intent of performing stochastic analyses that couple all pertinent fate and transport processes from the ground surface up to the 100-m point of assessment (POA).

This is a key component of the effort to include uncertainty quantification and sensitivity analysis (UQSA) in the next revision of the E-Area Performance Assessment (PA). This report describes the model and shows results obtained from benchmarking the model to best-estimate deterministic results obtained using the PORFLOW aquifer zone model. The PORFLOW model is three-dimensional (3D) while the GoldSim model represents a simplified one-dimensional (1D) treatment. Nevertheless, the GoldSim model was able to reproduce PORFLOW results, with acceptable accuracy, as shown in Table ES-1 below. One key calibration target is the prediction of a radionuclide's peak concentration value at the 100-m POA. Given the time windows established for many groundwater limits (e.g., ST-ET beta-gamma limits are currently set for three separate time periods), the timing of this peak is also of importance. For all of the parent radionuclide test cases evaluated, GoldSim predicted peak concentrations within 29% of the PORFLOW values and peak times agreed within 25% (with the majority of the results in better agreement). The behavior of the radionuclides modeled more closely matches that seen for the pulse tracer than for the steady-state tracer in terms of the peak value and timing. Therefore, initial calibration of the GoldSim model to the PORFLOW pulse tracer results was deemed to be the more appropriate target. The calibration did not produce consistent results for many of the radionuclide progeny, which is believed to be due to the complex hydrostratigraphy of the region below the ST06 footprint. Note that for Th-230, Ra-226, and Pb-210 (U-238 progeny), a peak concentration was not attained after 20,000 years. Reassessments will be made when the vadose zone GoldSim models are connected to the GoldSim aquifer model. Note that the parameter settings established are universal in nature and are independent of radionuclide and its progeny.

Table ES-1. Comparison of GoldSim and PORFLOW peak concentrations and times at the POA.

Nuclides	PORFLOW		GoldSim		%Difference	
	Max Concentration	Max Time	Max Concentration	Max Time		
	mol/L	Year	mol/L	Year	Concentration	Year
C-14	3.692E-09	18.2	4.353E-09	22.8	-18%	-25%
H-3	2.020E-08	4	1.738E-08	4.3	14%	-8%
I-129	4.133E-09	20.5	4.366E-09	22.8	-6%	-11%
Np-237	2.36E-09	54.2	1.675E-09	59.5	29%	-10%
U-233	1.139E-14	73.3	7.082E-16	8000	94%	>200%
Th-229	3.231E-18	5280	6.912E-18	14100	-114%	-167%
Sr-90	1.683E-10	64	1.424E-10	71.1	15%	-11%
Tc-99	6.173E-09	14	6.432E-09	15.4	-4%	-10%
U-238	1.985E-11	5100	1.789E-11	5500	10%	-8%
U-234	2.600E-17	14100	1.627E-17	6300	37%	55%
Th-230	1.878E-19	20000+	1.236E-19	20000+	34%	0%
Ra-226	2.002E-20	20000+	1.942E-24	20000+	100%	0%
Pb-210	1.000E-23	20000+	2.435E-28	20000+	100%	0%
Tracer (Pulse)	2.541E-08	4.2	2.219E-08	4.4	13%	-5%
Tracer (SS)[1]	1.000E-08	N/A	7.914E-09	11.6	21%	N/A

[1] SS – Steady-state

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

DU	Disposal Unit
ELLWF	E-Area Low-Level Waste Facility
GSA	General Separations Areas
POA	Point of Assessment
PA	Performance Assessment
SRNL	Savannah River National Laboratory
SRS	Savannah River Site
TCCZ	Tan Clay Confining Zone
UQSA	Uncertainty Quantification and Sensitivity Analysis
WSRC	Westinghouse Savannah River Company
1D	One-Dimensional
3D	Three-Dimensional
K_d	Radionuclide sorption coefficient

1.0 Introduction

This report presents the calibration of the E-Area Low-Level Waste Facility (ELLWF) GoldSim aquifer model. This is a key component of the effort to include uncertainty quantification and sensitivity analysis (UQSA) in this revision of the E-Area PA, considering recommendations from the 2015 PA strategic planning team outlined by Butcher and Phifer (2016).

As part of the Performance Assessment (PA) for the ELLWF, an assessment of uncertainty in the results and sensitivity to model parameters is necessary. Uncertainty analysis involves stochastic Monte Carlo calculations sampling distributions of model parameters and performing many individual model calculations that are subsequently statistically analyzed. Making many model simulations (typically 1,000 to 10,000) with the full three-dimensional (3D) PORFLOW models would be prohibitively time consuming. As an alternative, the approach taken for non-cementitious disposal units (DU) and underlying aquifer in this revision of the E-Area PA is to develop a one-dimensional (1D) model of flow and transport benchmarked to PORFLOW results and subsequently used to perform the requisite stochastic calculations in a reasonable amount of time. SRNL is using the GoldSim® software (GTG, 2018) to develop such models. Typically, making use of distributed processing, a Monte Carlo simulation with 10,000 realizations can be run in 10 to 20 hours depending on model complexity.

The aquifer model is a sub-model of the GoldSim system model described by Wohlwend (2020). GoldSim does not explicitly solve porous-media flow equations. It solves the transport equation typically expressed as a 1D model representation. For E-Area considerations, several aspects of the fate and transport of contaminants from the water table beneath a DU to the 100-m well are multidimensional in nature. Typically, streamtraces emanating into the aquifer at the water table surface are non-linear as they progress towards the downstream 100-m point of assessment (POA). Additional distortion among these streamtraces occur due to the potential presence of underlying clay layers. Therefore, GoldSim flow and transport results require calibration to the more realistic 3D PORFLOW aquifer model deterministic results. This calibration process provides a level of confidence that the GoldSim-based stochastic results are reliable.

The work presented herein documents the model development methodology and its application to the calibration of the aquifer zone portion of the model from below the Slit Trench #6 (ST06) footprint to the 100-m well. The calibration focuses on the maximum (peak) concentration and timing for a non-sorbing, non-decaying tracer and seven parent radionuclides: C-14, H-3, I-129, Np-237, Sr-90, Tc-99, and U-238. Np-237 and U-238 have progeny and their short-chain progeny were included within the analysis efforts.

The results obtained from benchmarking to best estimate PORFLOW results are presented. To capture 3D flow effects in a 1D model usually requires some adjustment to nominal model settings. In this case, better agreement between the two models was obtained by adjusting the nominal volumetric flow rate and plume parameter settings (i.e., a plume function was employed to address transverse spreading along the path lengths).

The ST06 location resides within the center set of Slit Trenches and contains the underlying Tan Clay Confining Zone (TCCZ) within the aquifer unit (see Figure 1-1). The vertical location of this clay layer places it in the direct transport path for many of the PORFLOW streamtraces prior to them reaching the 100-m POA. The TCCZ ranges in thickness from ~6 feet to ~22 feet (average about 12-to-15 feet) within E-Area and new Plot 8. Figure 1-2 shows a plot of the distance (feet) from the top of the water table to the top of the TCCZ. The red dashed line in the figure shows where these two surfaces cross. Negative numbers represent where the TCCZ surface resides in the vadose zone above the water table and positive numbers where the TCCZ resides in the aquifer. For footprints in the western sector of E-Area, this clay layer resides completely within the vadose zone, while for the eastern sector this clay layer resides deep enough into the aquifer to minimize its impact on streamline behavior. As such, the more challenging location within the center sector was chosen for model development. Therefore, the model developed and presented within this report is general enough to handle the other footprint conditions where geometric parameter adjustments will be required but no additional modelling components (e.g., no additional flow paths) are envisioned. Figure 1-1 shows the location of ST06 relative to the overall ELLWF facility layout.

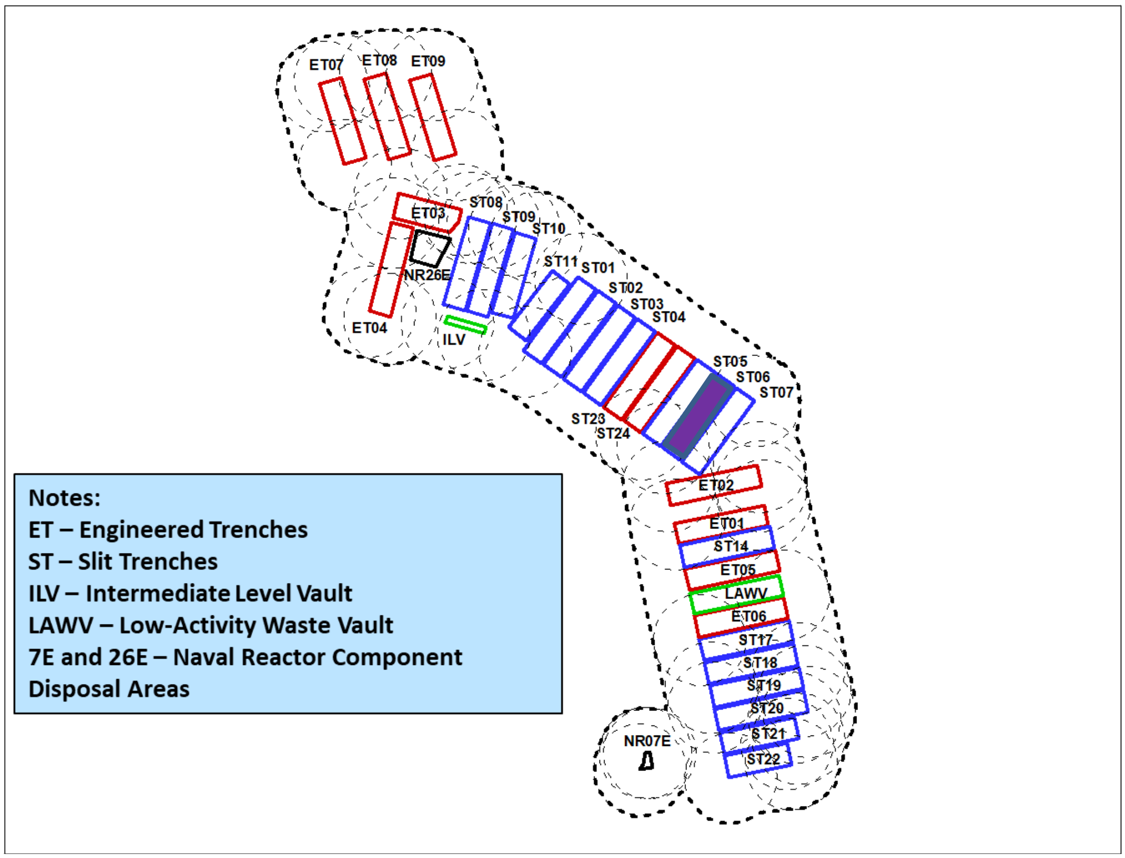

Figure 1-1. Layout of the ELLWF showing the location ST06 (purple).

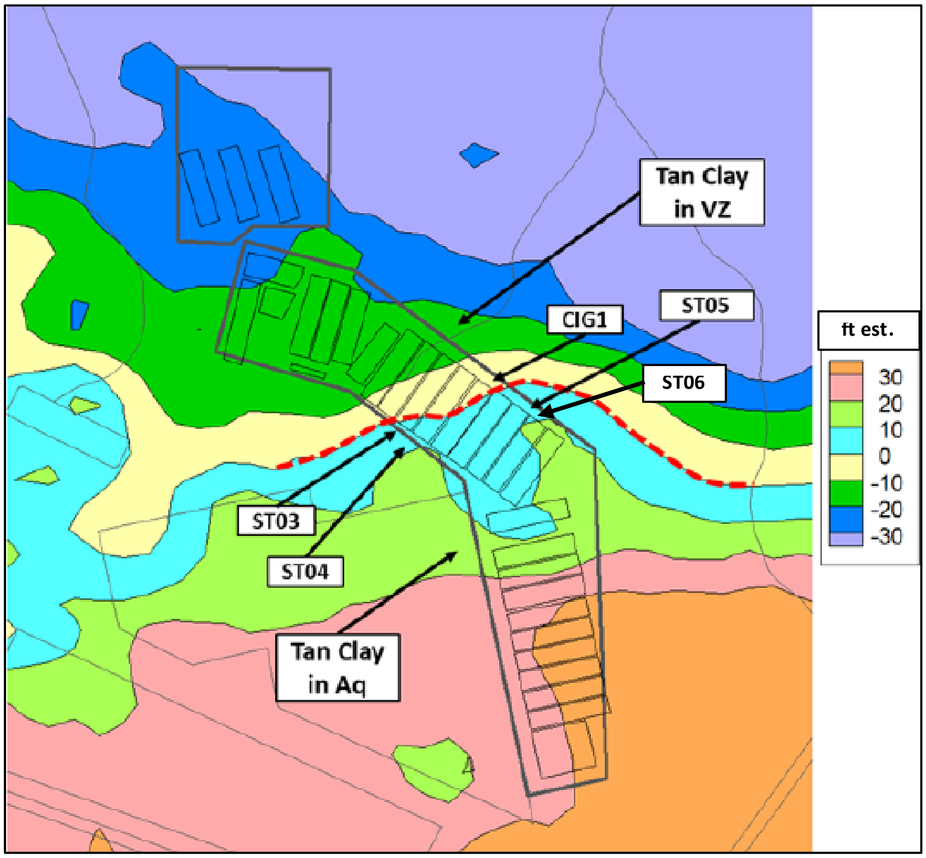

Figure 1-2. Plot of TCCZ position relative to Water Table.

2.0 Aquifer Model Description

The conceptual model of the aquifer zone is shown schematically in Figure 2-1. After transport through the upper and lower vadose zone, the radionuclides enter the aquifer at the surface of the water table. Flux of contaminants from the vadose zone is transferred to an aquifer pathway that represents the footprint below the vadose zone DU. Multiple aquifer pathways are then utilized to model the transport through the aquifer, ending at the 100-m POA.

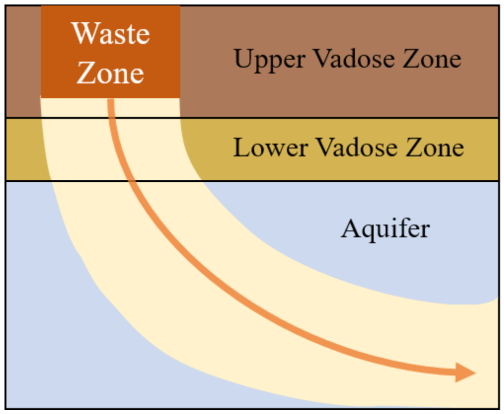

Figure 2-1. GoldSim ELLWF trench conceptual model.

To better understand groundwater flow through the aquifer below the ELLWF DUs, the flow fields from the 2018 General Separations Area (GSA) aquifer flow model (Flach 2018) were investigated. The flow field below the DUs is complex due to the multiple hydrostratigraphic layers as shown in Figure 2-2. The blue lines represent the flow through the aquifer (i.e., 3D streamtraces extracted from the 3D flow field), first going into the initial sandy layer (flow is almost horizontal) then passing through the green clay layer (almost vertical flow) and the second sandy layer (again flow is almost horizontal), finally passing through the tan clay layer (almost vertical flow). The ultimate discharge point for these streamtraces is the seepage faces associated with Upper Three Runs creek.

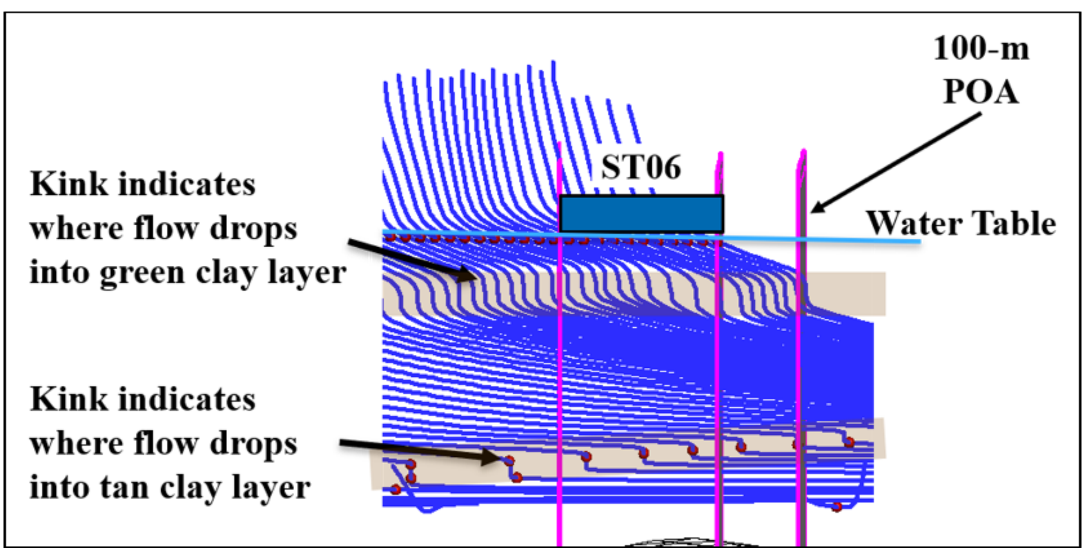

Figure 2-2. Flow fields under the ST06 DU from the 2018 GSA Aquifer Flow Model.

The flow through the aquifer can be represented by a GoldSim streamtube (Figure 2-3). The first section represents the flow through the initial sandy layer with flow area, A_1. The second represents the flow through the tan clay layer with flow area, A_2, and the final section represents the flow through the second sandy layer with flow area, A_3 (note that the flow directly under the ST06 footprint does not pass through the green clay layer before reaching the POA).

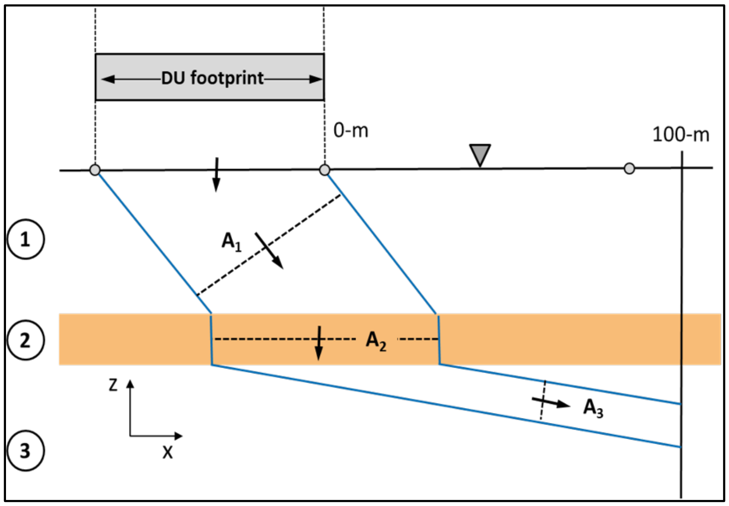

Figure 2-3. Streamtube representation of the flow through the aquifer.

Within a streamtube at steady-state flow:

$$Q = Q_1 = Q_2 = Q_3 \quad \textbf{(1)}$$

where

Q_i - volumetric flowrate of water through segment i (ft^3/yr)

These flowrates can be broken out as:

$$Q_i = A_i U_i = A_i \phi_i v_i \quad \textbf{(2)}$$

where

A_i - segment i cross-sectional total area (ft^2)

U_i - segment i Darcy velocity (ft/yr)

ϕ_i - segment i effective porosity (-)

v_i - segment i phasic velocity (ft/yr)

For GoldSim purposes, a simple 1D model (aligned with respect to the flow direction) is shown in Figure 2-4.

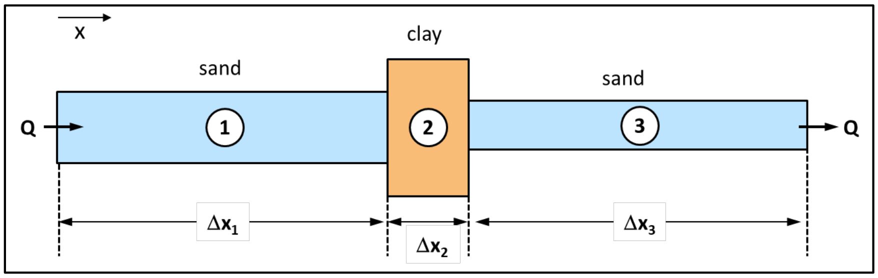

Figure 2-4. 1D model of a streamtube.

The PORFLOW aquifer model employs transverse dispersion which allows the contaminants to disperse laterally as well as in the longitudinal direction of flow (along a streamtube). As the contaminants laterally disperse, they can migrate into neighboring streamtubes which changes their flow path. For some contaminants (specifically those with high clay K_d values) this can cause significant amount of the concentration to bypass the clayey layer and travel along the sandy layer just above the clay layer to the POA (i.e., short-circuiting the more highly retarded flow path). This can be seen in the PORFLOW concentration profiles shown in Figure 2-5. As time progresses contaminants begin reaching the POA from successively lower points on the POA.

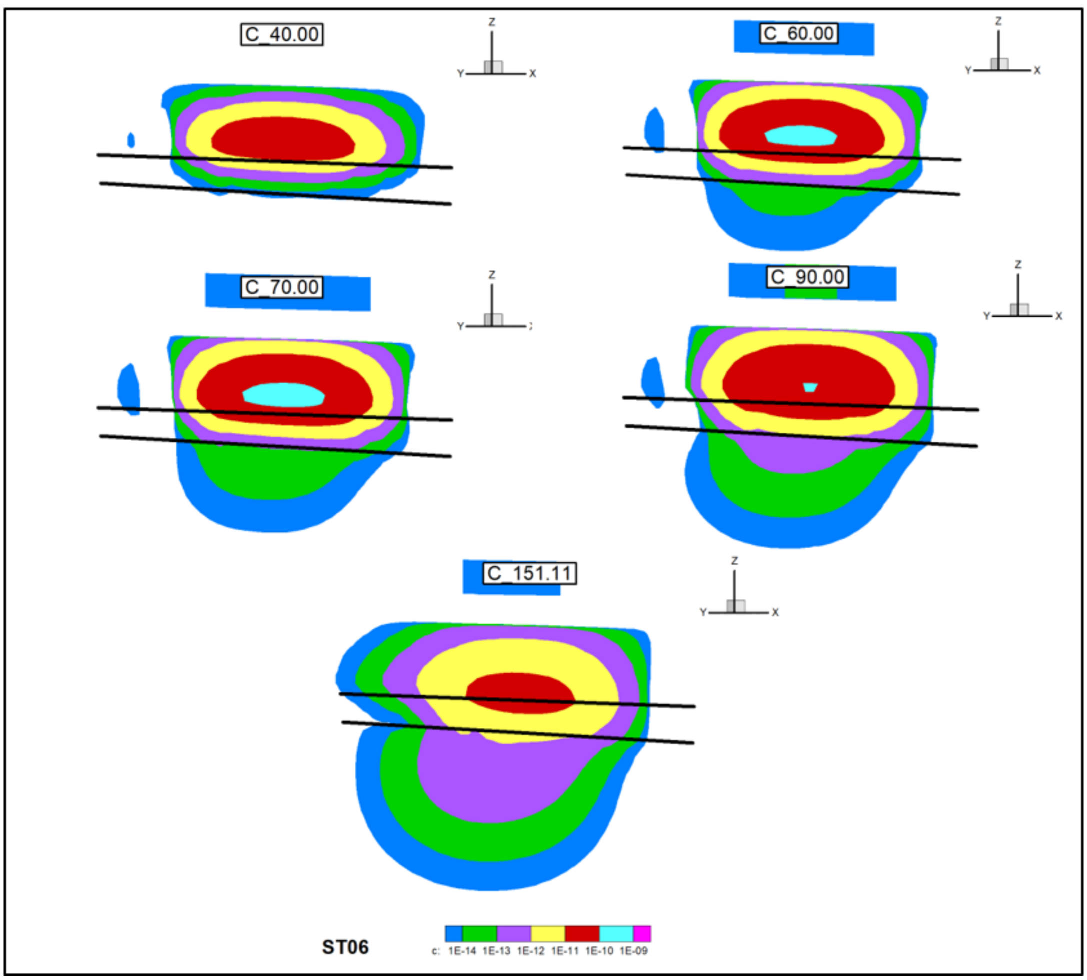

Figure 2-5. PORFLOW-based Sr-90 concentration profiles at the POA through time.

This effect is also seen in the concentration plot where the maximum concentration at the POA is made up of multiple peaks. The initial (largest) peak is from a location (node) above the clayey layer. As you shift to different nodes, the depth increases and the maximum concentration location goes into the tan clay layer and then into the sandy layer below, this is shown in Figure 2-6.

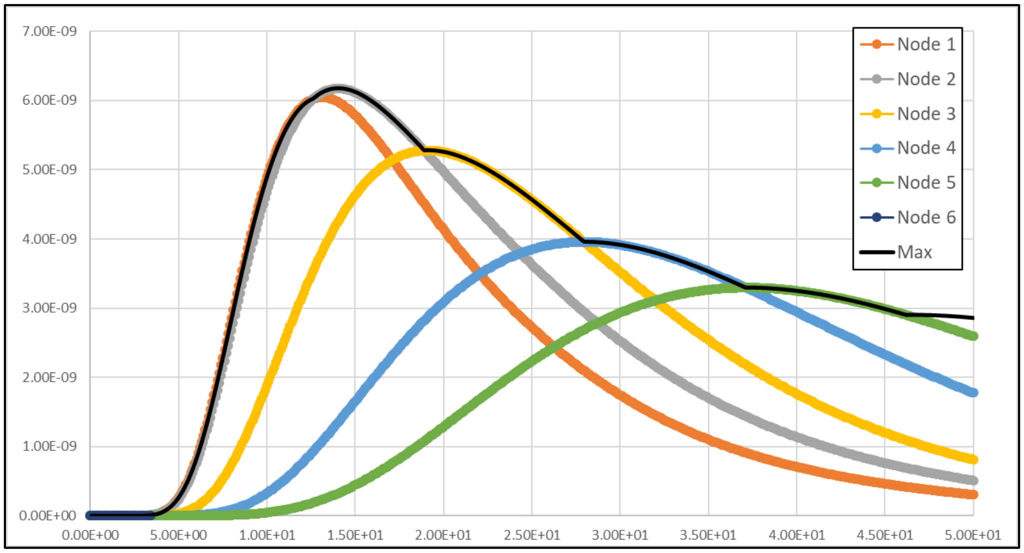

Figure 2-6. PORFLOW-based Concentration (mol/L) vs Time (yr) at the POA for Tc-99.

In order to better model this 3D behavior in the 1D GoldSim model, two aquifer flow paths are utilized as shown in Figure 2-7:

- The top path models the flow above the clayey layer, traveling only through the initial sandy layer above the clay layer. This transport path results from a combination of partial lateral flows and lateral dispersion that is occurring above the clay layer; and
- The bottom path represents the flow that passes through the clayey layer into the lower sandy layer before reaching the POA. This transport path corresponds directly with the streamtubes generated from the PORFLOW flow model and is a direct result of advection.

The splitting of contaminant between these two paths and each path's timing to reach the POA can be understood based on the chemical absorption (K_d) properties of the elements. A listing of their values is presented in Table 2-1. The overall impact is consistent with the magnitude of the retardation ratio between clay versus sand.

Table 2-1. Key transport properties of the chemical elements considered.

Nuc	Half-life (yr)	Sand Kd	Clay Kd	Sand R	Clay R	Clay/Sand R ratio
Tracer	na	0	0	1	1	1.0
H-3	1.23E+01	0	0	1	1	1.0
U-238	4.47E+09	300	400	1252	1669	1.3
Tc-99	2.11E+05	0.6	1.8	3.5	8.5	2.4
I-129	1.57E+07	1	3	5.2	13.5	2.6
Np-237	2.14E+06	3	9	13.5	38.5	2.9
Sr-90	2.89E+01	5	17	21.9	71.9	3.3
C-14	5.70E+03	1	30	5.2	126.1	24.4

In GoldSim each flow path is made up of aquifer pathway elements representing the different zones within each path.

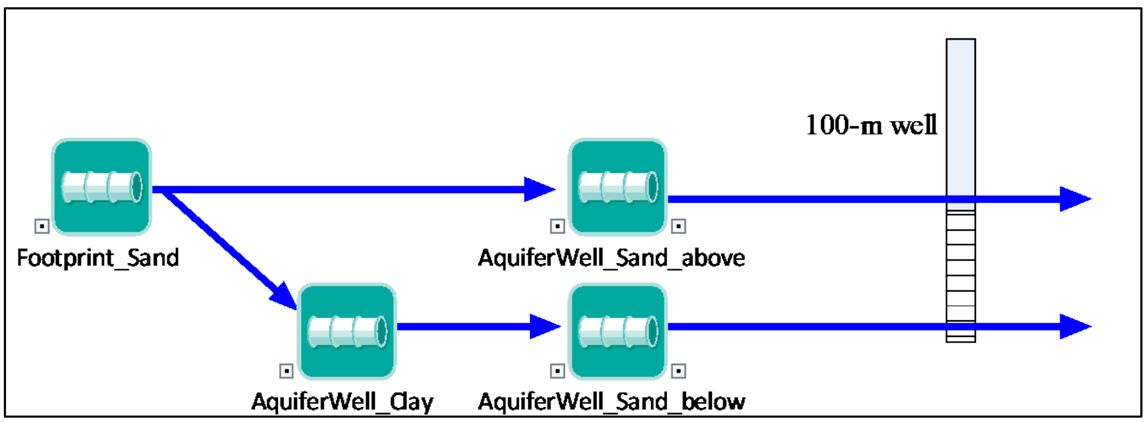

Figure 2-7 GoldSim representation of the Aquifer Zone.

The conceptual model implemented within the aquifer pathway element is a row of linked computational cells having no-flow boundaries on the top, bottom and sides, allowing 1D transport solely in the aquifer flow direction. The “Footprint_Sand” element represents the area directly below the DU footprint (first streamtube section) while the “AquiferWell_Clay” and “AquiferWell_Sand_above” and “AquiferWell_Sand_below” elements represent the portion of the aquifer pathway that is comprised of clayey and sandy (above the clayey layer and below the clayey layer) soils, respectively. Each aquifer element contains several transport and geometric parameters to simulate the entire aquifer zone. The “Footprint_Sand” element also contains a source region where the inventory is uniformly placed. An example of the aquifer pathway and the transport and geometric parameters utilized is shown in Figure 2-8. The initial volumetric flow rate (315.08 ft^3/d) is estimated using the phasic velocity (0.011 ft/d), area (117,629 ft^2), and porosity (0.25) calculated in the clayey region by the GSA aquifer flow model. To calibrate to the PORFLOW targets, the volumetric flow rate of the streamtube below the clayey layer was reduced by 50% (157.6 ft^3/d).

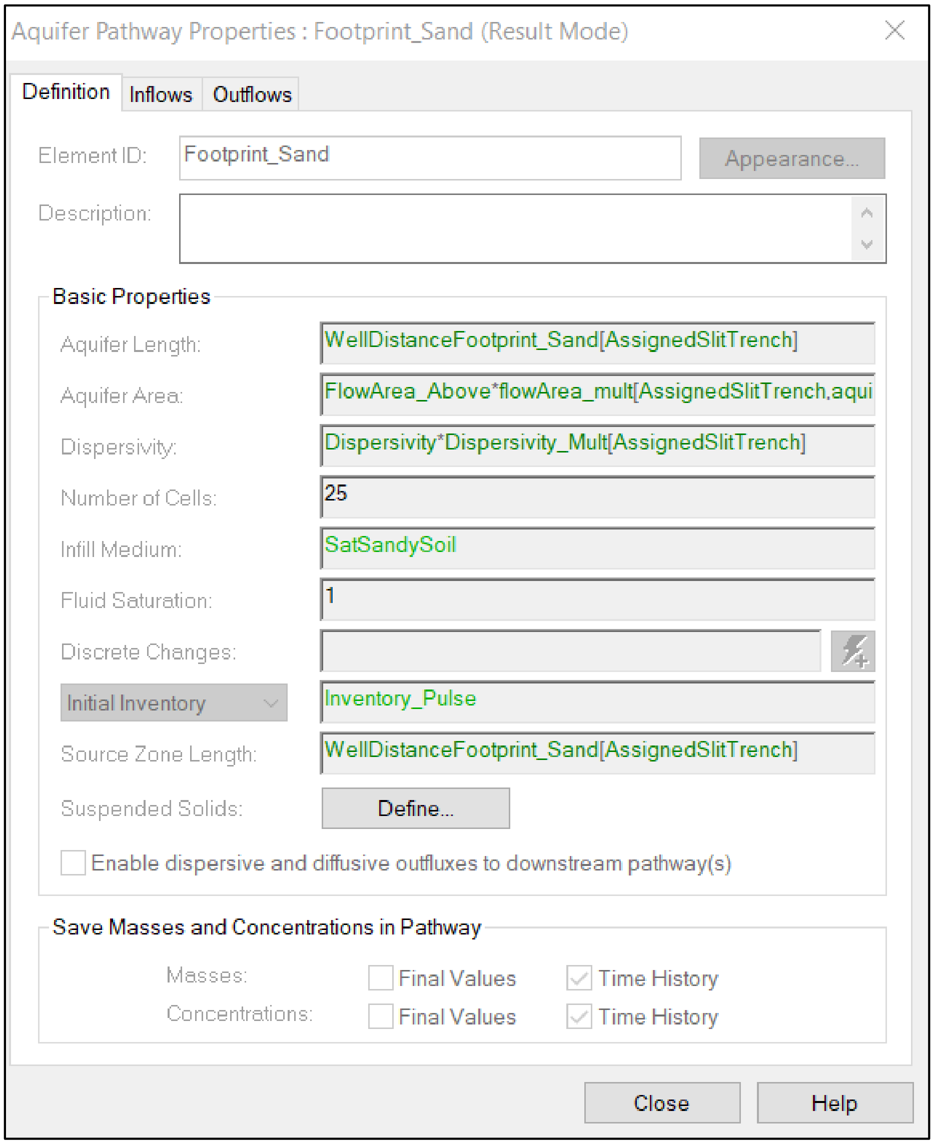

Figure 2-8. "Footprint" region aquifer pathway dialog box showing transport and geometric parameters.

Each aquifer pathway element defines the length, area, dispersivity, number of cells, the infill medium, saturation, and inventory (if applicable) of the pathway. The infill medium sets the porosity and density of the medium as well as chooses the K_d of each element. The aquifer length and area of each pathway is estimated from PORFLOW streamtrace data and is given in Table 2-2.

Table 2-2. Geometric parameters of aquifer pathway elements.

	Footprint Sand	Sand Above	Clay	Sand Below
Flow Path Length (m)	130.18	100	5.23	87.49
Plume Width (m)	51.82	0.00	51.82	51.82
Plume Height (m)	8.58	7.48	210.90	6.37
Flow Area (m^2)	444.7	444.7	10928.1	330.1

Because GoldSim models 1D flow, the concentration of each aquifer element outflow represents the average concentration and 3D spatial variation is not represented. This is conceptually different from the PORFLOW 3D aquifer model that accounts for spatial variation, vertical and transverse diffusion and reports the maximum concentration at each position along the POA boundary. To be consistent with the PORFLOW transport simulations, a plume function is applied to the POA concentration. The plume function allows the 1D model to represent transverse and vertical dispersion within the aquifer from the source to the POA that is handled explicitly in the 3D PORFLOW model.

The plume function has eleven input arguments that account for the spatial variation (Tauxe 2019) and produces a multiplier that varies between zero and one. The eleven arguments used in the plume function are given in Table 2-3, and Figure 2-9 is a schematic that illustrates the physical meaning of many of the arguments. The pathway length (X_L) varies depending on the aquifer section and is estimated using the predicted distance traveled from PORFLOW streamtraces (Table 2-2). The aquifer cross-sectional area (A) of each section is the same and is based on half of the average width and height of the sandy aquifer zones as measured in PORFLOW (193.7 m). The length of the source parallel to the flow direction (L_S) is half of the length of the total disposal unit length. The top of the source is assumed to be at ground surface therefore the vertical depth to the top of the source from the top of the aquifer (D_S) is 0 m. The vertical distance between the ground surface to the observation point (X_V) is 0 m for the streamtube above the clayey layer and 8.58 m for the streamtube below the clayey layer. The transverse position of the observation point (X_T) is set to 0 m. The width of the source, transverse to the aquifer flow (W_S), is set to the width of the disposal unit. The thickness of the source (b_S) is set to 0 m. The thickness of the aquifer (b) is set to the average sandy zone height as measured in PORFLOW, (7.48 m). The transverse and vertical dispersivity is set to 1.54 m. In addition to the plume function, a peaking factor of 1.2 (20%) was applied to the streamtube below the clayey layer to better match the PORFLOW steady-state tracer results

Table 2-3. 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]
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

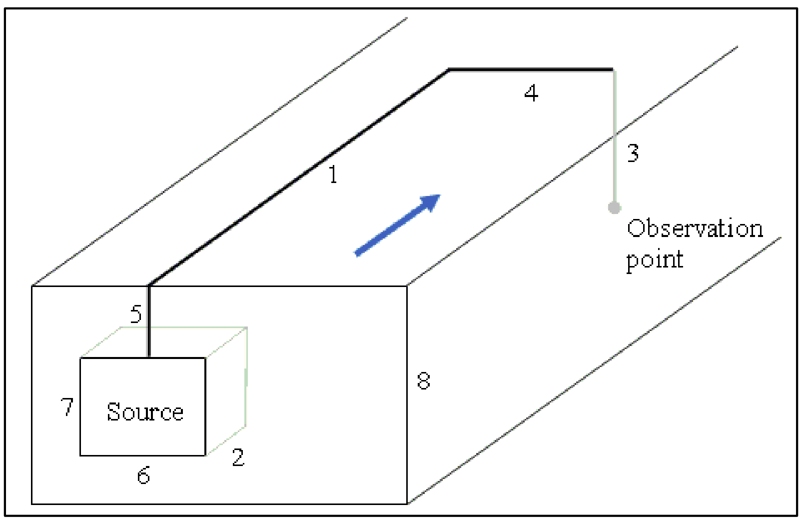

Figure 2-9 Schematic representation of the plume function.

2.1 Dashboard User Interface

The home screen of the ELLWF Trench System Model is shown in Figure 2-10. Choosing the "Home Dashboard" link accesses the home dashboard (Figure 2-11) where the user can move to the model switches and trench dashboards (Figure 2-12 and Figure 2-13, respectively). In the model switches dashboard, the user can choose to allow retardation, institutional control, and diffusion. This dashboard also controls the subsidence parameters that are used in the vadose zone portion of the model. The trench dashboard allows the user to select which trench to model as well as inventory parameters.

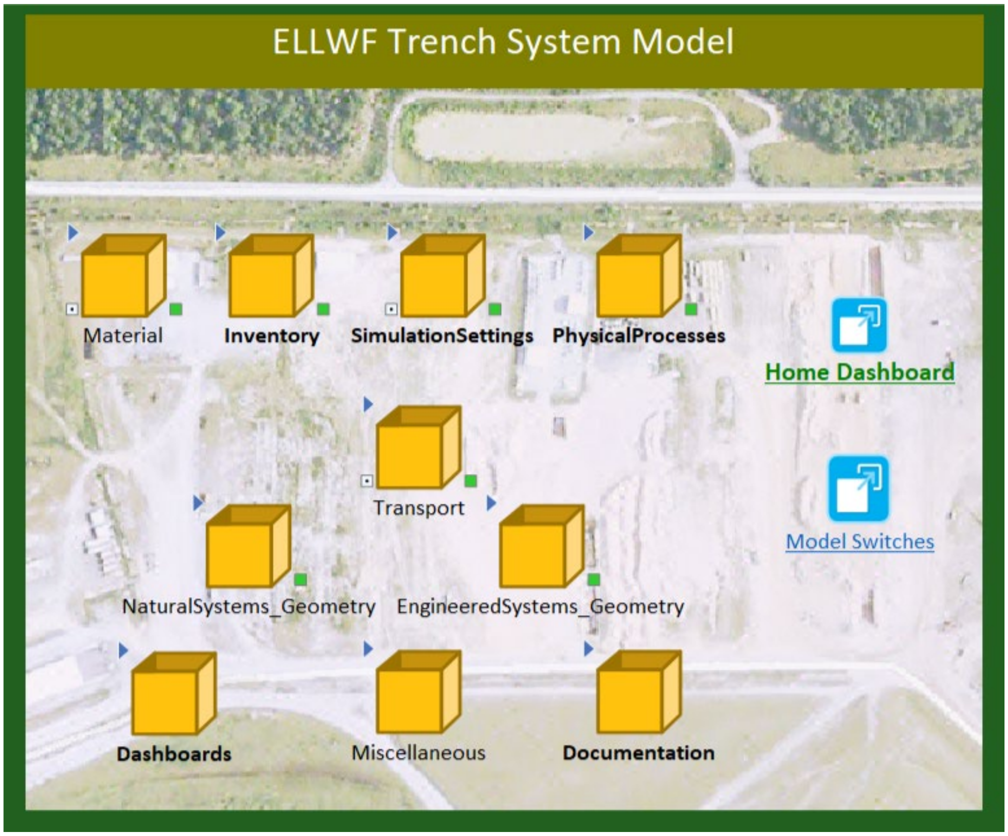

Figure 2-10. Top-Level container of the GoldSim System Model.

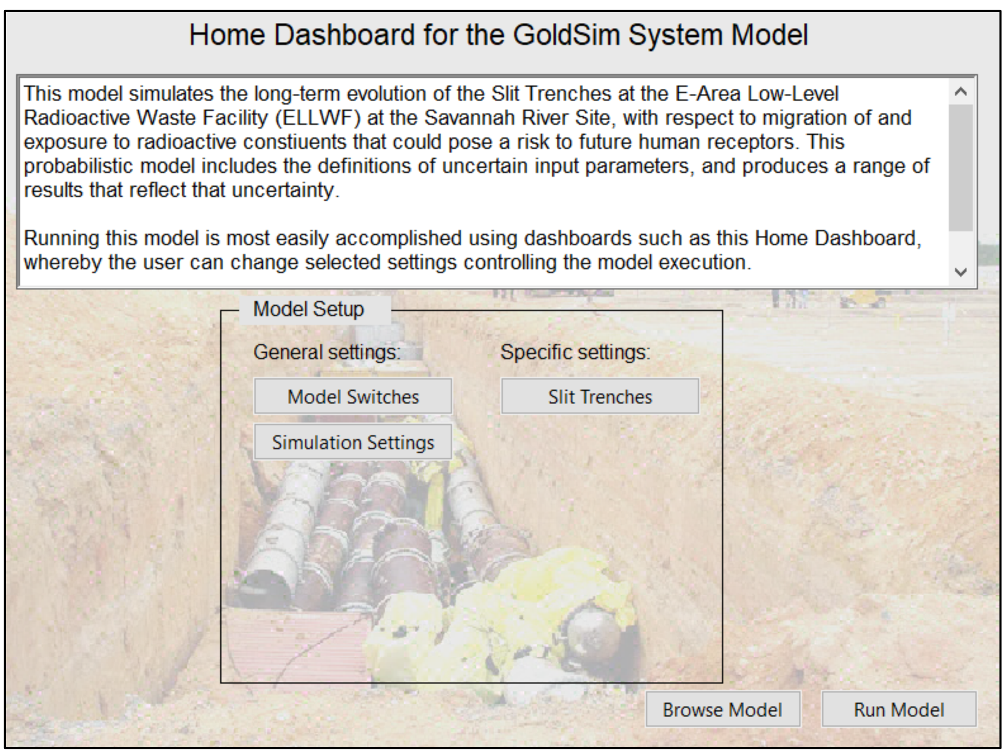

Figure 2-11. GoldSim System Model home dashboard.

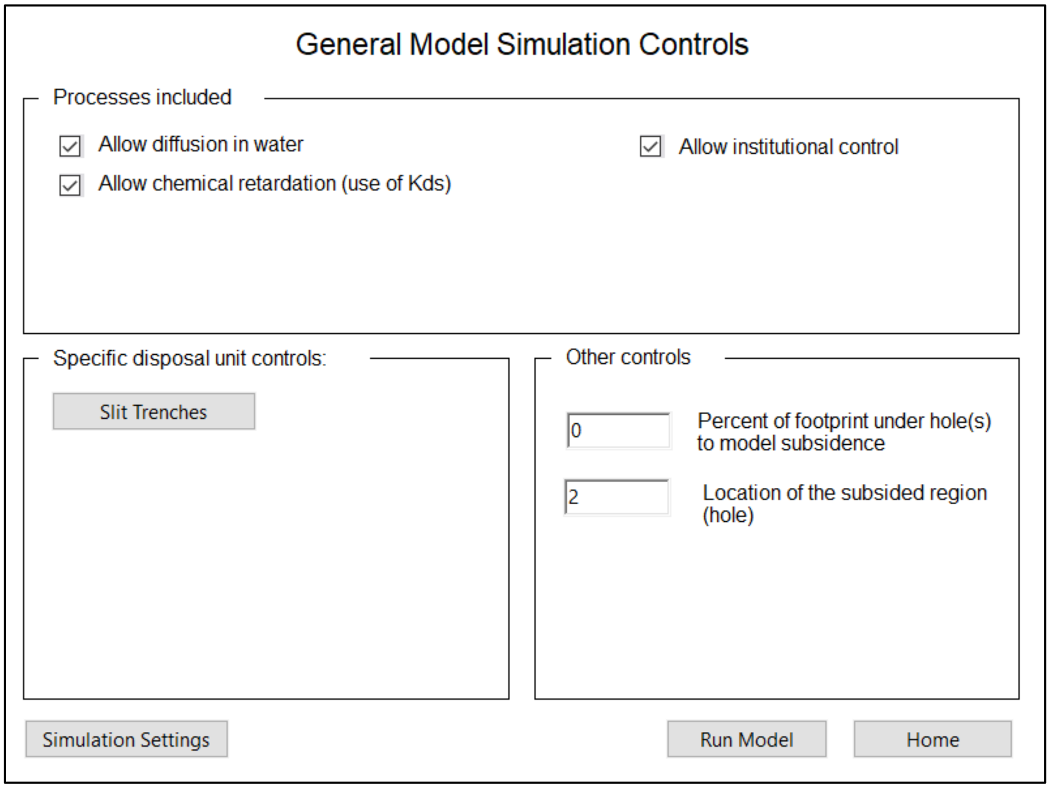

Figure 2-12. GoldSim System Model general simulation dashboard.

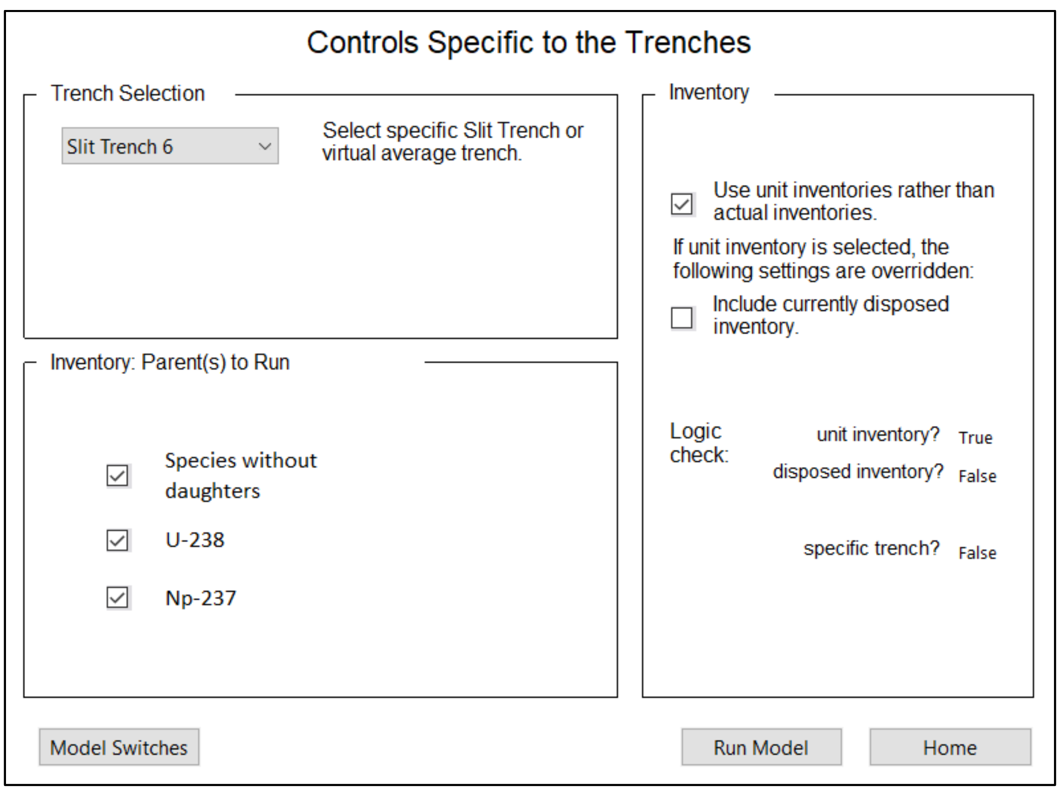

Figure 2-13. Dashboard to choose trench specific parameters.

2.2 Material, Chemical and Radionuclide Properties

A significant amount of hydraulic properties data exists for the GSA and is contained in a configuration-controlled data package (Nichols and Butcher 2020). Pertinent data from this source have been transferred into the GoldSim aquifer model. Figure 2-14 shows the contents of the GoldSim Materials container including definitions of contaminant species and their decay rates, and the material properties of the physical materials making up the solid porous and fluid media. Table 2-4 lists nominal values for the saturated soil material properties used in the GoldSim Aquifer model obtained from Nichols and Butcher (2020). Water content is the product of porosity and saturation.

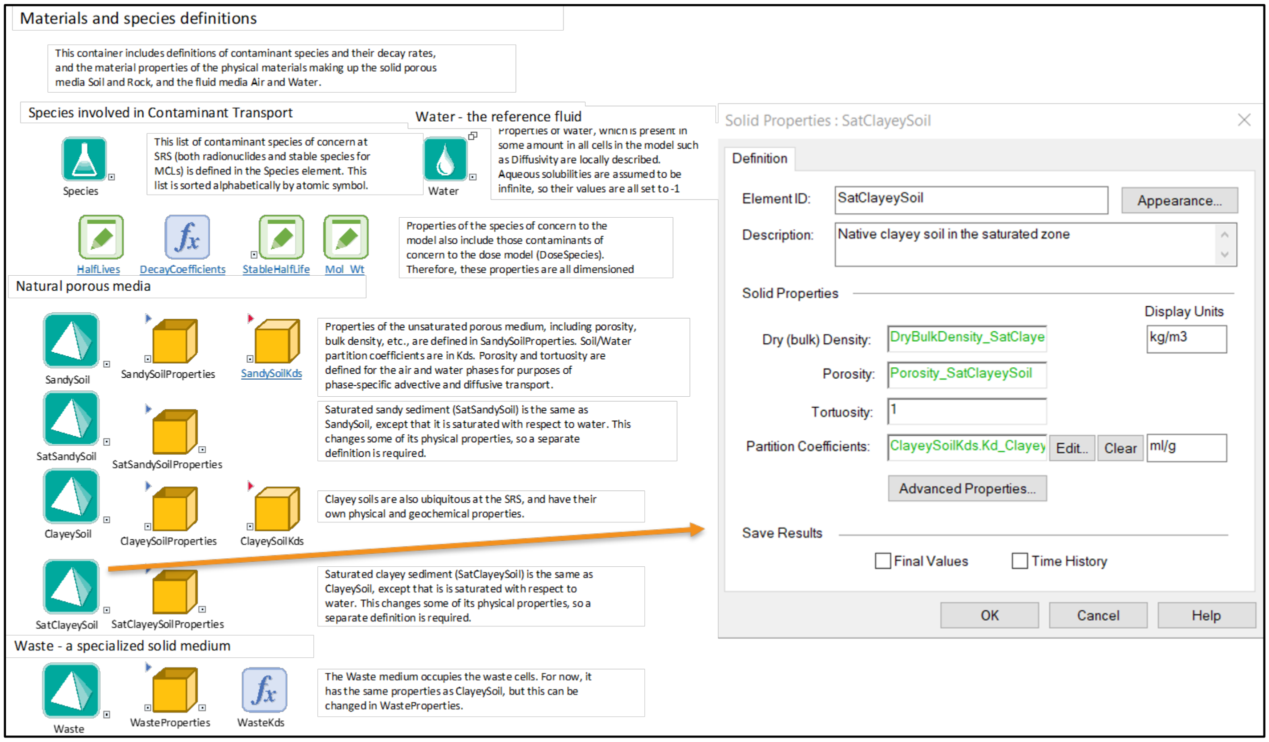

Figure 2-14. Contents of materials container and SatClayeySoil material definition.

Table 2-4. Soil material properties used in the GoldSim Aquifer model.

Material	Dry Bulk Density (g/cm^3)	Porosity	Effective Diffusion Coefficient (cm^2/yr)
SatSandySoil	1.04	0.250	1.67E+02
SatClayeySoil	1.04	0.250	1.26E+02

Geochemical data used in the GoldSim aquifer model is from a configuration-controlled data package produced by Kaplan (2016). Figure 2-15 shows the contents of the GoldSim Geochemical container where radionuclide partition coefficients (i.e., K_d values) for the soil materials are defined. The saturated sandy and clayey soils have the same partition coefficients as their unsaturated counterparts. Table 2-5 lists nominal values for the chemical properties used in the GoldSim Aquifer model obtained from Kaplan (2016).

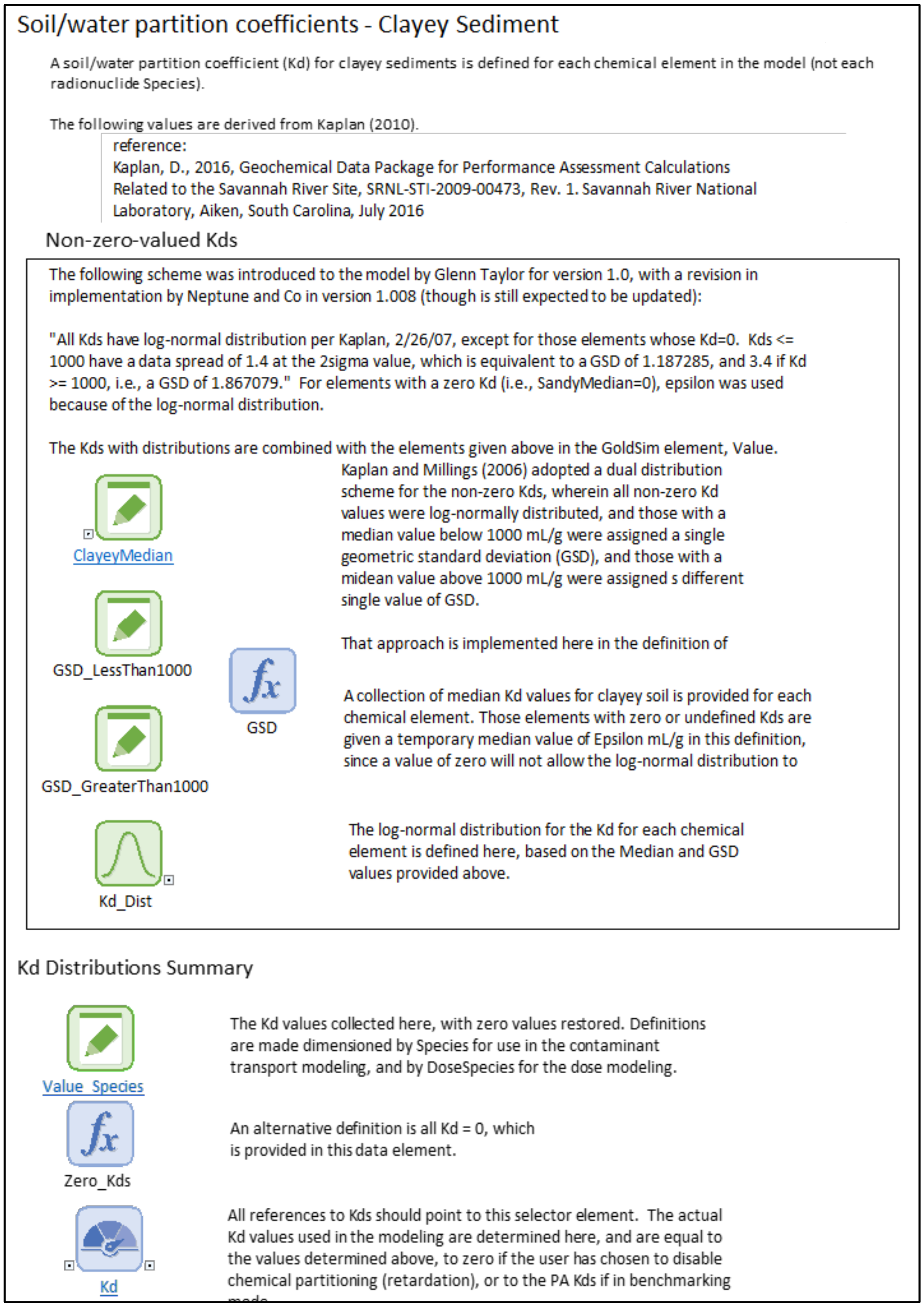

Figure 2-15. Contents of Clayey soil geochemical container where model chemical properties are defined.

Table 2-5. 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

Radionuclide data used in the GoldSim aquifer model is from a configuration-controlled data package produced by Smith et al. (2019). Radionuclide half-life and decay data for the species included in the model calibration are defined in the Material container (Figure 2-14). Table 2-6 lists nominal values for the radionuclide properties used in GoldSim vadose zone modeling obtained from Smith et al. (2019).

Table 2-6. Radionuclide data for species modeled.

Species ID	Atomic Weight (g/mol)	Half-life (year)	Progeny
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
U-233	233	1.59E+05	Th-229
Th-229	229	7.34E+03	
Sr-90	90	2.88E+01	
Tc-99	99	2.11E+05	
U-238	238	4.47E+09	U-234
U-234	234	2.46E+05	Th-230
Th-230	230	7.54E+04	Ra-226
Ra-226	226	1.60E+03	Pb-210
Pb-210	210	2.22E+01	

3.0 Model Benchmarking to PORFLOW

The PORFLOW 3D Aquifer Flow and Transport Model is utilized to estimate initial aquifer geometric parameters and Darcy velocity as well as provide target concentration profiles for calibration. For benchmarking, a tracer (no retardation or decay) is placed at the water table under the DU. Figure 3-1 shows the results of the benchmarking of the GoldSim Aquifer model to the PORFLOW tracer results. The output reports the maximum concentration value of the concentrations along the 100-m curtain for PORFLOW and the maximum concentration from either the path above the tan clay or the path below the tan clay (see Figure 2-7). At different timesteps, this could result in the maximum concentration being at different locations along the curtain. The kinks within the PORFLOW and GoldSim results indicate where the maximum concentrations at the POA go from above the tan clay confining layer to the sandy region below shown previously in Figure 2-6. For the pulse tracer results, GoldSim predicts a concentration history where the maximum concentration transitions from above the clayey layer to below at approximately 6 years. PORFLOW predicts a more complex time history with multiple peaks. This is a consequence of the complex hydrostratigraphy below the DU. The percent difference between GoldSim and PORFLOW concentration results is 21% for steady-state and 13% for pulse. These differences are sufficiently close for demonstration purposes.

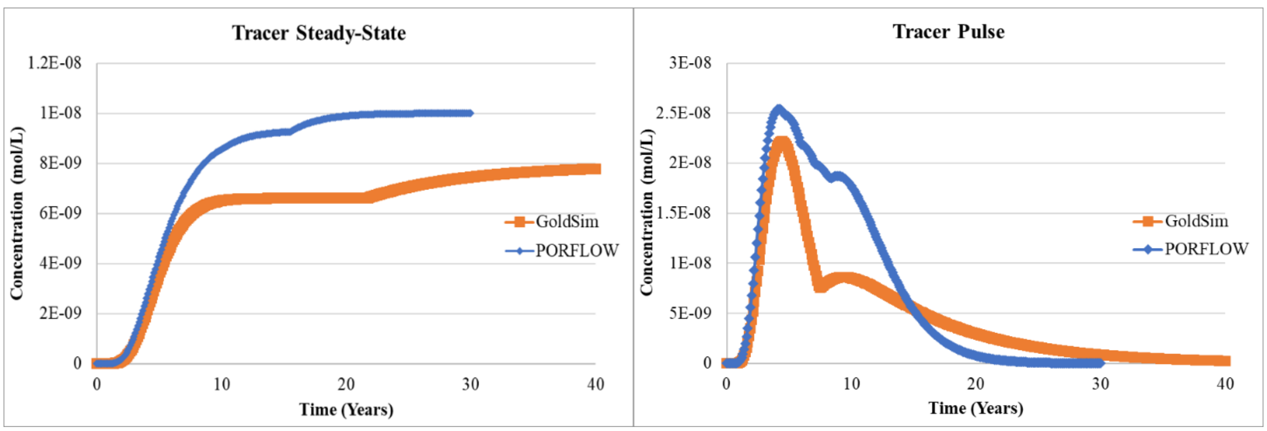

Figure 3-1. Pulse and Steady-State tracer concentration profiles for GoldSim and PORFLOW.

In addition to tracer simulations, 1 mole of each parent radionuclide is included in the source term of the footprint aquifer pathway to evaluate model calibration. The results of aquifer model calibration for the five parent radionuclides without progeny are shown in Figure 3-2. The calibration results for the Np-237 chain is shown in Figure 3-3 and the U-238 chain in Figure 3-4. Noticeable kinks are found in the PORFLOW concentration profiles which coincide with maximum concentration at different nodes along the POA curtain. By using two streamtubes in the 1D GoldSim model to represent the complex hydrostratigraphy below the DU, some of this kinking behavior is predicted yet underestimated as seen in the graphs. There are no kinks found in Sr-90 because the concentration below the clayey layer is always less than the concentration predicated above the clayey layer. The maximum concentrations and the time of the highest peak predicted by both PORFLOW and GoldSim are listed in Table 3-1. Note that for Th-230, Ra-226, and Pb-210 (U-238 progeny), a peak concentration was not attained after 20,000 years. The maximum absolute percent difference for the parent radionuclides is found to be 29% for Np-237. This is believed to be due to the difference between the sandy and clayey K_d values (Table 2-5) which further complicates the 3D to 1D abstraction in addition to the complex hydrostratigraphy below the ST06 footprint.

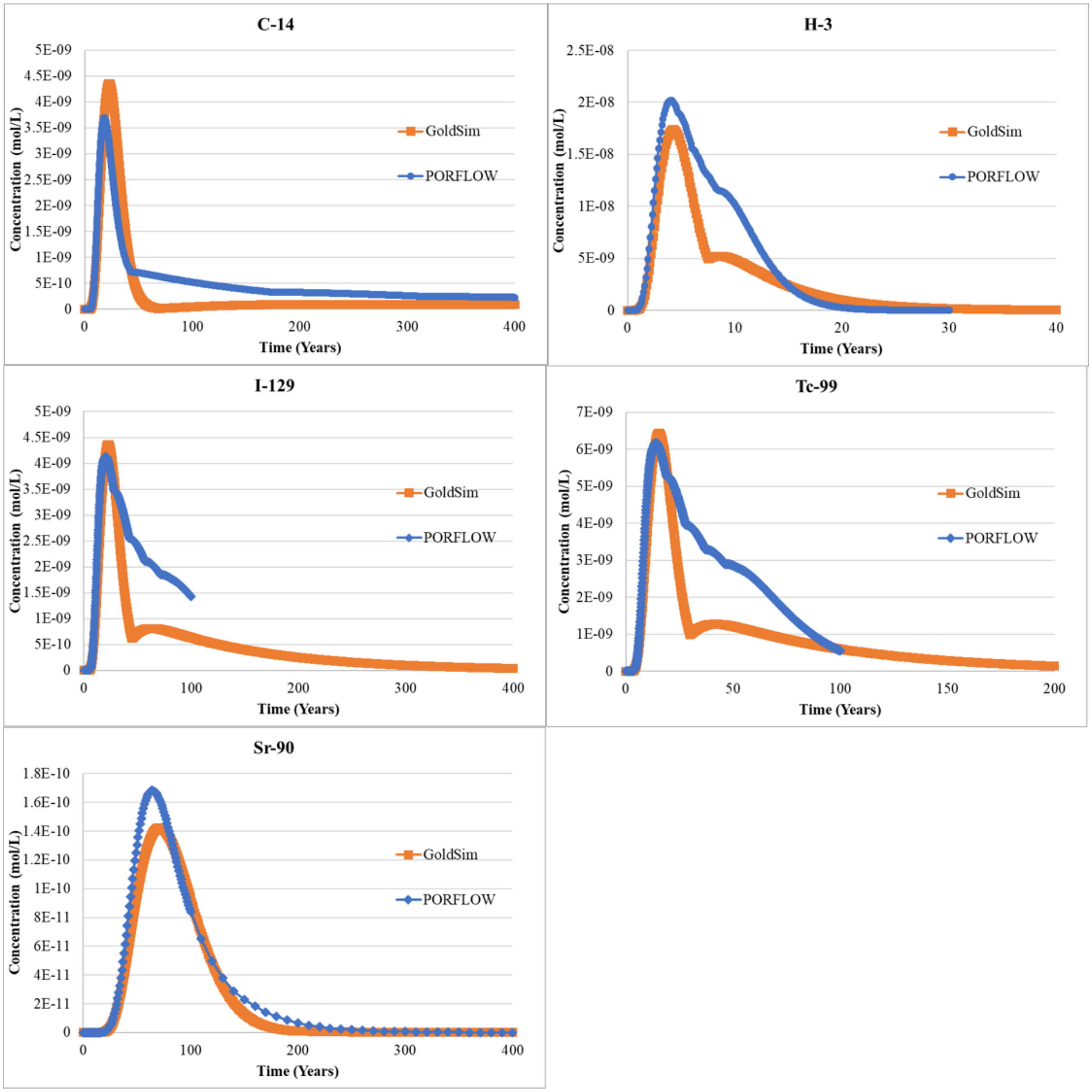

Figure 3-2. Concentrations at the 100-m POA predicted by GoldSim and PORFLOW for radionuclides without progeny.

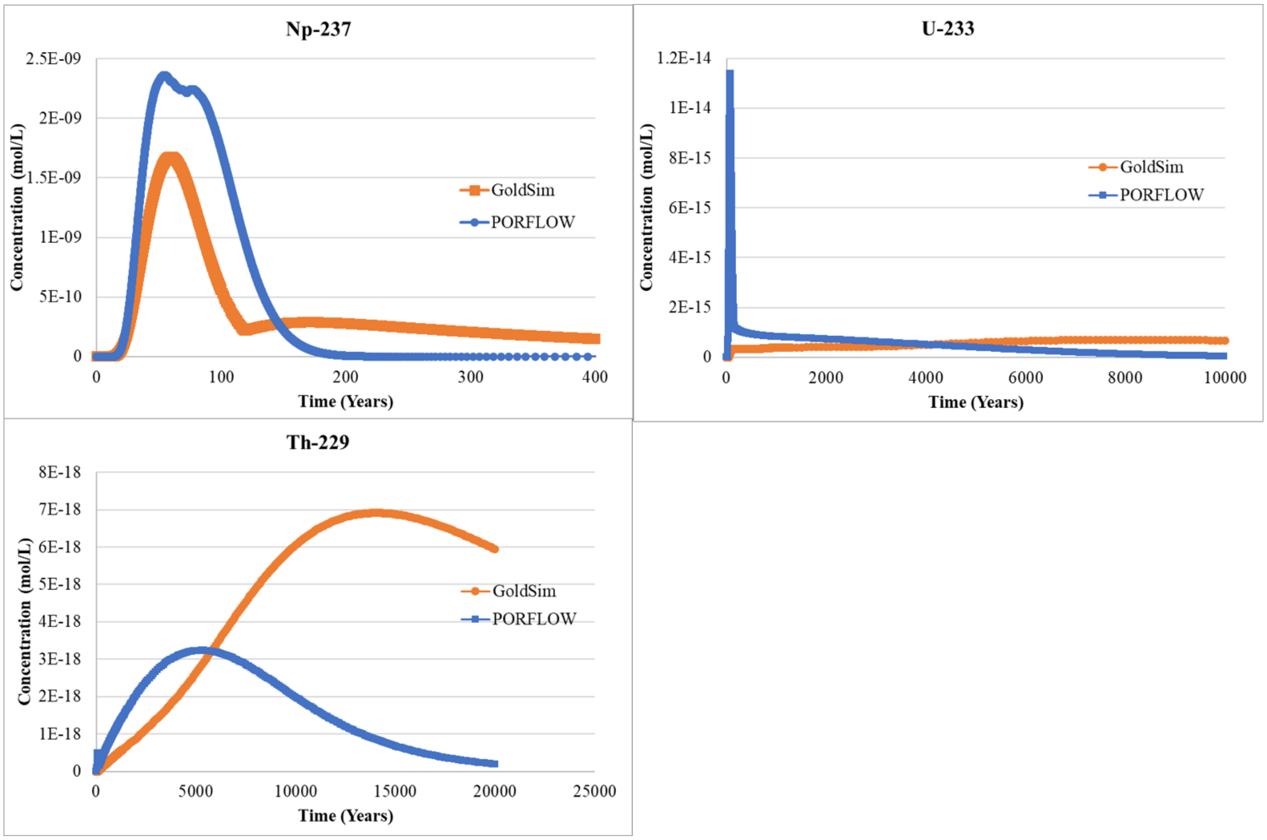

Figure 3-3. Concentrations at the 100-m POA predicted by GoldSim and PORFLOW for the Np-237 chain.

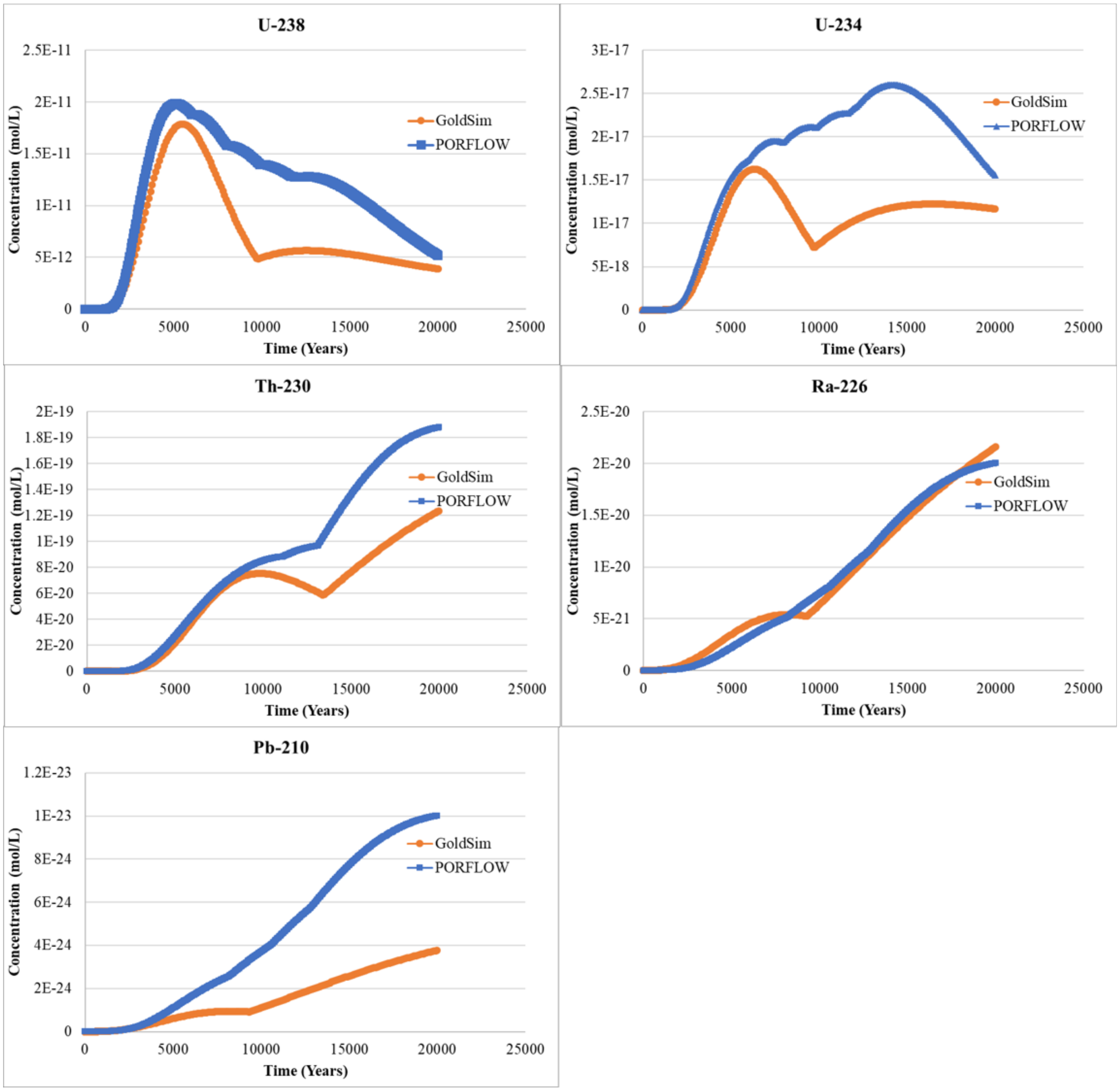

Figure 3-4. Concentrations at the 100-m POA predicted by GoldSim and PORFLOW for the U-238 chain.

Table 3-1. Comparison of GoldSim and PORFLOW peak concentrations and times at the POA.

Nuclides	PORFLOW		GoldSim		%Difference	
	Max Concentration	Max Time	Max Concentration	Max Time		
	mol/L	Year	mol/L	Year	Concentration	Year
C-14	3.692E-09	18.2	4.353E-09	22.8	-18%	-25%
H-3	2.020E-08	4	1.738E-08	4.3	14%	-8%
I-129	4.133E-09	20.5	4.366E-09	22.8	-6%	-11%
Np-237	2.36E-09	54.2	1.675E-09	59.5	29%	-10%
U-233	1.139E-14	73.3	7.082E-16	8000	94%	>200%
Th-229	3.231E-18	5280	6.912E-18	14100	-114%	-167%
Sr-90	1.683E-10	64	1.424E-10	71.1	15%	-11%
Tc-99	6.173E-09	14	6.432E-09	15.4	-4%	-10%
U-238	1.985E-11	5100	1.789E-11	5500	10%	-8%
U-234	2.600E-17	14100	1.627E-17	6300	37%	55%
Th-230	1.878E-19	20000+	1.236E-19	20000+	34%	0%
Ra-226	2.002E-20	20000+	1.942E-24	20000+	100%	0%
Pb-210	1.000E-23	20000+	2.435E-28	20000+	100%	0%
Tracer (Pulse)	2.541E-08	4.2	2.219E-08	4.4	13%	-5%
Tracer (SS)[1]	1.000E-08	N/A	7.914E-09	11.6	21%	N/A

[1] SS – Steady-state

A pulse tracer is more relevant to the case where inventory is introduced instantaneously into a DU with no engineered barriers. Therefore, initial calibration of the GoldSim model to the PORFLOW pulse tracer result was deemed to be the more appropriate target. As can be seen in Table 3-1 and the preceding Figure 3-3 the behavior of these parent radionuclides more closely matches that seen for the pulse tracer than for the steady-state tracer in terms of the peak value and timing. The set of radionuclides selected for these runs include a wide range of sorption values (Table 2-5) and half-lives (Table 2-6) anticipated in the larger list of parent radionuclides expected to be important contributors to dose in the PA. The calibration did not produce consistent results for many of the radionuclide progeny, which is believed to be due to the complex hydrostratigraphy of the region below the ST06 footprint. Reassessments will be made when the vadose zone GoldSim models are connected to the GoldSim aquifer model. Given additional effort, the parameter settings could be adjusted to produce more agreement between PORFLOW and GoldSim results. However, the parameter settings that were chosen, give comparable results over a wide range of sorption values and half-lives.

4.0 Conclusions

A 1D GoldSim model has been developed to model the transport of radionuclides through the aquifer zone to the 100-m POA for ST06. The model calculates the maximum concentration at the POA for parent and progeny radionuclides. During the development of the GoldSim Aquifer model, results from the PORFLOW GSA flow model were investigated thoroughly and it was found that the flow below ST06 is complex due to the presence of multiple hydrostratigraphic layers. In order to better estimate the complex 3D behavior, two streamtubes were employed in the 1D GoldSim Aquifer model.

Results from PORFLOW transport simulations were used to benchmark the GoldSim model. Complete results from this code-to-code benchmarking are provided in Section 3.0 of this report. GoldSim model results were found to be comparable to those obtained by PORFLOW. The volumetric flow rate for both streamtubes as well as the plume function parameters were investigated. It was found that modifying the volumetric flow rate of the region below the clayey layer and utilizing a peaking factor for the concentrations in that region produced the lowest percent difference between PORFLOW and GoldSim. As shown in Figure 2-6, PORFLOW results for many of the radionuclides include multiple kinks in the concentration history due to the maximum concentration moving deeper in the aquifer as time increases. Typically, it is difficult to reproduce 3D flow effects with a 1D model and, in that respect, results of this benchmarking study are very good. The calibration did not produce consistent results for many of the radionuclide progeny, which is believed to be due to the complex hydrostratigraphy of the region below the ST06 footprint. Note that for Th-230, Ra-226, and Pb-210 (U-238 progeny), a peak concentration was not attained after 20,000 years. Reassessments will be made when the vadose zone GoldSim models are connected to the GoldSim aquifer model.

The GoldSim model is intended to be used for Monte Carlo analysis to determine uncertainty in radionuclide concentrations at the 100-m POA. Ultimately, the GoldSim Aquifer model will be connected to the vadose zone via mass transfer from the bottom of the DU to the footprint pathway element.

5.0 References

Butcher and Phifer, 2016. B. T. Butcher and M. A. Phifer, *Strategic Plan for Next E-Area Low-Level Waste Facility Performance Assessment*. SRNL-STI-2015-00620, Revision 0. February 2016.

Flach 2019. G. P. Flach, *Updated Groundwater Flow Simulations of the Savannah River Site General Separations Area*, SRNL-STI-2018-00643, Revision 0, Savannah River National Laboratory, Aiken, South Carolina, January 2019.

GTG 2018. *GoldSim® User's Guide Version 12.1*. GoldSim® Technology Group. Issaquah, WA. June 2018.

Kaplan 2016. D. I. Kaplan, *Geochemical Data Package for Performance Assessment Calculations Related to the Savannah River Site*, SRNL-STI-2009-00473, Revision 1, Savannah River National Laboratory, Aiken, South Carolina, August 2016.

Nichols and Butcher 2020. R. L. Nichols and B. T. Butcher, *Hydraulic Properties Data Package for the E-Area Soils, Cementitious Materials, and Waste Zones – Update*, SRNL-STI-2019-00355, Revision 1, Savannah River National Laboratory, Aiken, South Carolina, May 2020.

Smith et al. 2019. F. G. Smith, III, B. T. Butcher, L. L. Hamm, W. P. Kubilius, *Dose Calculation Methodology and Data for Solid Waste Performance Assessment and Composite Analysis at the Savannah River Site*, SRNL-STI-2015-00056, Revision 1, Savannah River National Laboratory, Aiken, South Carolina, August 2019.

Tauxe, 2019. J. D. Tauxe, *Notes on the GoldSim Plume Function*. Neptune and Company, Inc. Los Alamos, NM. August 2019.

Wohlwend, 2020. J. L. Wohlwend, *E-Area Low-Level Waste Facility GoldSim System Model*. SRNL-STI-2020-00079, Revision 0. April 2020.

Distribution:

cj.bannochie@srnl.doe.gov
alex.cozzi@srnl.doe.gov
a.fellinger@srnl.doe.gov
samuel.fink@srnl.doe.gov
brenda.garcia-diaz@srnl.doe.gov
connie.herman@srnl.doe.gov
dennis.jackson@srnl.doe.gov
brady.lee@srnl.doe.gov
patricia.lee@srnl.doe.gov
joseph.manna@srnl.doe.gov
daniel.mccabe@srnl.doe.gov
gregg.morgan@srnl.doe.gov
frank.pennebaker@srnl.doe.gov
amy.ramsey@srnl.doe.gov
william.ramsey@SRNL.DOE.gov
eric.skidmore@srnl.doe.gov
michael.stone@srnl.doe.gov
boyd.wiedenman@srnl.doe.gov
terry.foster@srnl.doe.gov
Records Administration (EDWS)

sebastian.aleman@srnl.doe.gov
tom.butcher@srnl.doe.gov
kerri.crawford@srs.gov
thomas.danielson@srnl.doe.gov
kenneth.dixon@srnl.doe.gov
james.dyer@srnl.doe.gov
peter.fairchild@srs.gov
scott.germain@srs.gov
luther.hamm@srnl.doe.gov
thong.hang@srnl.doe.gov
daniel.kaplan@srnl.doe.gov
dien.li@srs.gov
steven.mentrup@srs.gov
verne.mooneyhan@srs.gov
ralph.nichols@srnl.doe.gov
virginia.rigsby@srs.gov
jansen.simmons@srs.gov
frank.smith@srnl.doe.gov
ira.stewart@srs.gov
tad.whiteside@srnl.doe.gov
jennifer.wohlwend@srnl.doe.gov