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).

Disclaimer:

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 Modeling of Vadose Zone Transport for E-Area Naval Reactor Component Disposal Areas: Model Description and Benchmarking

F. G. Smith, III

July 2020

SRNL-STI-2020-00214, Revision 0

SRNL.DOE.GOV

DISCLAIMER

Printed in the United States of America

Prepared for
U.S. Department of Energy

SRNL-STI-2020-00079
Revision 0

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

Retention: *Permanent*

GoldSim Modeling of Vadose Zone Transport for E-Area Naval Reactor Component Disposal Areas: Model Description and Benchmarking

F. G. Smith, III

July 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:

____

F. G. Smith, III, Environmental Modeling, SRNL Date

TECHNICAL REVIEW:

____

S. E. Aleman, Environmental Modeling, SRNL Date

____

B. T. Butcher, Environmental Modeling, SRNL Date

APPROVAL:

____

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

EXECUTIVE SUMMARY

This report documents the development of a GoldSim® model of flow and radionuclide transport to the water table through the Naval Reactor Components Disposal Area (NRCDA) waste disposal sites and underlying vadose zones. The model is designed to be used for Monte Carlo uncertainty analysis in support 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 a PORFLOW model of NRCDA vadose zone transport. The PORFLOW model is three-dimensional while the GoldSim model is a simplified one-dimensional treatment. Nevertheless, the GoldSim model was able to accurately reproduce PORFLOW results with some adjustment to the nominal dispersion coefficient and vadose zone flow area used as "tuning" parameters. An example of the results obtained comparing GoldSim and PORFLOW calculation of releases of I-129, Tc-99, C-14 and Ni-59 from waste disposal containers at the 643-26E site is shown in Figure 1 below. For all of the test cases evaluated, GoldSim predicted peak concentrations within 6% of the PORFLOW values and peak times agreed within 8% with the majority of the results in better agreement. The close agreement between the two models provides confidence that GoldSim will give results accurately reflecting the behavior of releases from the NRCDA under off-normal operating conditions for sensitivity and uncertainty analysis

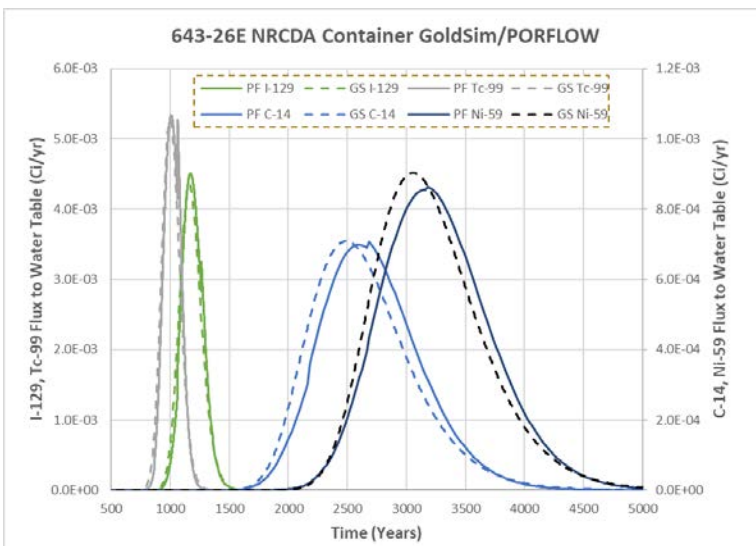

Figure 1. Comparison of GoldSim and PORFLOW results for release of radionuclides from bolted containers disposed in NRCDA 643-26E.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

ELLWF	E-Area Low-Level Waste Facility
GSA	General Separations Areas
HELP	Hydrologic Evaluation of Landfill Performance
IC	Institutional Control
LAZ	Lower Aquifer Zone
LVZ	Lower Vadose Zone
NR	Naval Reactor
NRCDA	Naval Reactor Component Disposal Area
PA	Performance Assessment
SRNL	Savannah River National Laboratory
SRS	Savannah River Site
TCZ	Tan Clay Zone
UVZ	Upper Vadose Zone
WSRC	Westinghouse Savannah River Company
WZ	Waste Zone
VZ	Vadose Zone

1.0 Introduction

A PORFLOW model of infiltration and radionuclide transport through the waste region and underlying vadose zone at the Naval Reactor Component Disposal Area (NRCDA) disposal sites has been developed (Hang and Hamm, 2019). This model will be used to calculate fluxes to the water table from radionuclide releases at the NRCDA sites. These fluxes provide input to a separate PORFLOW model of groundwater flow in the aquifer beneath the NRCDA disposal sites that will calculate radionuclide concentrations at points of assessment (POA) along the aquifer. Concentrations will be converted into the dose received by members of the public from exposure to the radionuclides through various pathways. The PORFLOW models are three-dimensional and as such can take a significant amount of time to calculate results particularly for radionuclides having decay chains where multiple isotopes must be tracked.

As part of the Performance Assessment (PA) for the E-Area Low Level Waste Facility (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 PORFLOW models would be prohibitively time consuming. As an alternative, the approach taken for non-cementitious disposal units in this revision of the E-Area PA is to develop a one-dimensional model of flow and transport benchmarked to PORFLOW results and subsequently use this model to perform the requisite stochastic calculations in a reasonable amount of time. SRNL is using the GoldSim® software (GoldSim Technology Group, 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.

In this report, a GoldSim model of flow and transport through the NRCDA vadose zone is described and the results obtained from benchmarking to best estimate PORFLOW results are presented. To capture three-dimensional flow effects in a one-dimensional model usually requires some adjustment to nominal model settings. In this case, better agreement between the two models was obtained by adjusting the nominal dispersion coefficient and slight modification of the flow area.

2.0 Naval Reactor Component Disposal Areas

The NRCDA is composed of two separate sites 643-7E and 643-26E located in E-Area as shown in Figure 2.1.1 (Hamm, 2019). The sites are at-grade level gravel pads where Naval Reactor (NR) waste containers are placed for permanent disposal. Site 643-7E was opened as an NR waste storage area in 1987. The site was reclassified as a disposal area in 2004 and the 41 NR containers on the pad at that time declared as disposed in-place (Wilhite and Flach, 2004). In 2005, soil was mounded over the 41 containers and the site closed to future disposal. Disposal site 643-26E was opened in 1997 and is still in operation. It is estimated that 33 heavily shielded, welded carbon steel casks and over 400 thinner-walled bolted containers will be disposed at this site before closure in 2065. Table 2.1.1 gives area footprints and nominal side lengths (assuming a square area) for the NRCDA sites (Hang and Hamm, 2019). As Figure 2.1.1 shows, the NRCDA sites do not have square footprints; however, using square side dimensions to approximate the shape of the disposal sites was deemed adequate for modeling purposes.

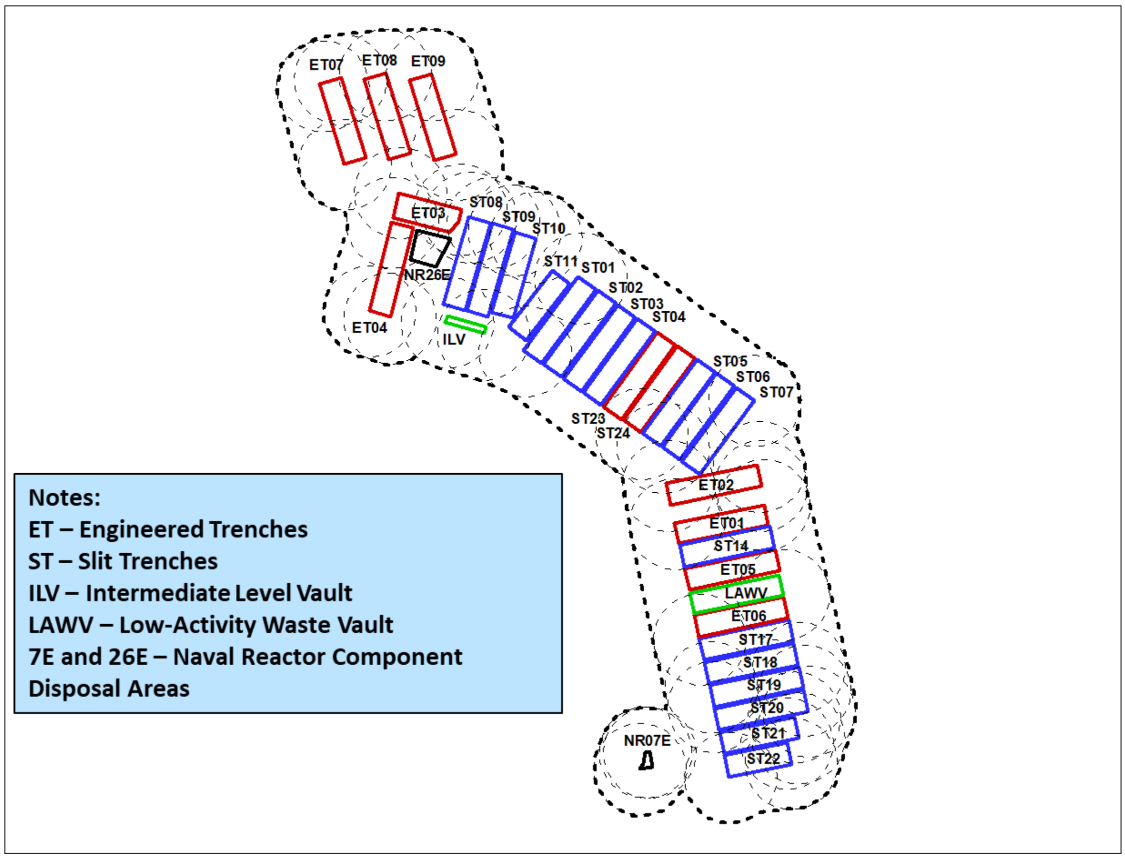

Figure 2.1.1 Location of NRCDA 643-26E (NR26E) and 643-7E (NR07E) in ELLWF.

Table 2.1.1 NRCDA Site Dimensions

Dimension	643-26E	643-7E
Area (ft^2)	47687	5878
Length (ft)	218.375	76.67

2.1 NRCDA Waste Characteristics

As described in the last PA (WSRC, 2008), NR waste consists of two general types: 1) highly radioactive components consisting of contaminated corrosion-resistant metal alloys and 2) auxiliary equipment contaminated with activated corrosion products. The more contaminated NR waste is contained in thick steel casks that are assumed to remain watertight for 750 years (Wohlwend and Butcher, 2018) after which corrosion and release of the waste material begins. Less contaminated NR waste is contained in thinner walled bolted containers that are assumed to either fail hydraulically when soil is mounded over the disposal pad or to also remain hydraulically sealed for 750 years (i.e., an early and late container failure timeline assumption).

Activated waste components in the steel casks are assumed to be a mixture of Inconel and Zircaloy having the corrosion rates listed in Table 2.1.2 (Yu et al., 2002). The total corrosion rate is calculated as:

$$C_T = f_I\, C_I + f_Z\, C_Z = f_I\, C_I + (1 - f_I)\, C_Z \tag{1}$$

where: C_T .... Total corrosion rate (1/yr)
f_I .... Inconel mass fraction in metal
f_Z .... Zircaloy mass fraction in metal $(1 - f_I)$
C_I .... Inconel corrosion rate (1/yr)
C_Z .... Zircaloy corrosion rate (1/yr)

It is assumed that the contamination is evenly distributed between the metal alloys according to their relative masses when both are present. The release rate of isotope *i* from the metal is then calculated as:

$$R(t)_i = C_T\, I(t)_i \tag{2}$$

where: $R(t)_i$............ Release rate at time t (Ci/yr)
$I(t)_i$............ Inventory (Ci) of isotope *i* in activated metal at time t

Although the model can accept any mixture of Inconel and Zircaloy, when applying these equations for the NRCDA corrosion rate, we would employ the two endpoints (i.e., f_I = 1 or 0 and, conversely, f_Z = 0 or 1).

Following hydraulic failure of the containment vessel, the model must account for parent decay and daughter in-growth within the remaining waste material as contamination is released at the corrosion rate calculated by Eq. (2). Release from bolted containers is somewhat simpler in that the model must only account for parent decay and daughter ingrowth until the contamination is released. Release of the entire waste inventory from bolted containers is assumed to occur instantaneously when the container fails.

Table 2.1.2 Corrosion Rates of NRCDA Metal Alloys

Metal Alloy	Corrosion Rate (1/yr)
Inconel	6.2194e-05
Zircaloy	9.7167e-06

2.2 NRCDA Vadose Zone Hydro-stratigraphic Layers

Figure 2.2.1 shows a generalized one-dimensional schematic diagram of an NRCDA disposal site and the underlying vadose zone hydro-stratigraphic layers. Figure 2.2.1 represents the true configuration of the 643-26E site while at the 643-7E site, which lies further east, the tan clay confining zone falls below the water table and the vadose zone consists of only the UVZ and LVZ layers. However, a vadose zone structure equivalent to that shown in Figure 2.2.1 can be used to generalize the GoldSim model for both sites. Dimensions of the zones for both NRCDA disposal sites (Bagwell and Bennett, 2018) and specification of soil material in the GoldSim model are listed in Table 2.2.1.

The above-grade waste disposal area is modeled as 18 ft deep when carbon steel casks are analyzed and 4.1 ft deep for a single layer of bolted containers. Bolted containers may be stacked to increase disposal capacity and the GoldSim model is able to use a waste thickness representing one, two, or three layers of waste containers.

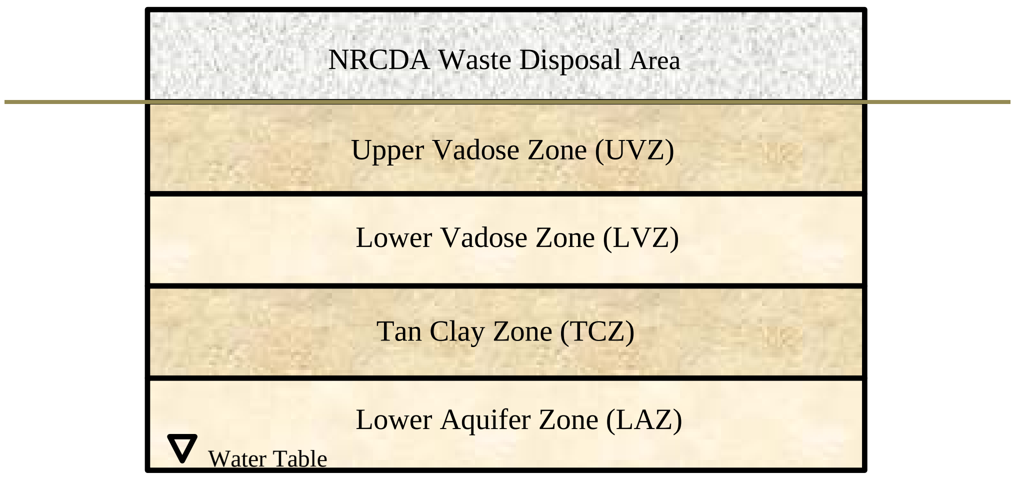

Figure 2.2.1 Schematic representation of NRCDA waste disposal site and vadose zone hydro-stratigraphic layers.

Table 2.2.1 Nominal Thickness in Feet and Composition of NRCDA Vadose Zone Segments

Vadose Zone Segments	643-26E (ft)	643-7E (ft)	643-7E (Modeled as Equivalent 4-Layer Vadose Zone)
Average Depth to Water Table	75 ft	63 ft	63 ft
UVZ	18 ft Clay	36 ft Clay	36 ft Clay
LVZ	39 ft Sand	27 ft Sand	9 ft Sand
TCZ	8 ft Clay	0	9 ft Sand
LAZ	10 ft Sand	0	9 ft Sand

2.3 NRCDA Timeline

Waste storage at NRCDA 643-7E was started prior to its designation as a disposal site and prior to waste disposal in 643-26E. Therefore, as described in documentation of the PORFLOW NRCDA model (Hang and Hamm, 2019), events at the two disposal sites follow different timelines. To facilitate software maintenance and quality assurance, it is highly desirable to have a single GoldSim model that can be used for either site. Therefore, the timeline information for both disposal sites was combined into the composite timeline shown in Table 2.3.1. The PORFLOW model report (Hang and Hamm, 2019) provides more detailed information about the timelines given in Table 2.3.1; however, event timings shown in this table are enough to construct the GoldSim model.

Table 2.3.1 Composite NRCDA Timeline

<table>
<tr><th>Calendar Date</th><th>Absolute Time (Numerical Calendar Date)</th><th>Time from Start of NRCDA Operations</th><th>643-7E Events</th><th>643-26E Events</th></tr>
<tr><td>1/1/1987</td><td>1987.003</td><td>0</td><td>First waste container placed.[1] Start radionuclide decay and daughter ingrowth.</td><td></td></tr>
<tr><td>9/28/1994</td><td>1994.743</td><td>7.740</td><td colspan="2">Start of ELLWF operations.</td></tr>
<tr><td>9/28/1997</td><td>1997.743</td><td>10.740</td><td></td><td>First waste container placed.[1] Start radionuclide decay and daughter ingrowth.</td></tr>
<tr><td>9/27/2005</td><td>2005.740</td><td>18.737</td><td>Soil mounded over waste containers. Hydraulic failure of bolted containers.[2]</td><td></td></tr>
<tr><td rowspan="2">9/28/2065</td><td rowspan="2">2065.743</td><td rowspan="2">78.740</td><td colspan="2">End of ELLWF operations.
Start of institutional control.</td></tr>
<tr><td></td><td>Soil mounded over waste containers. Hydraulic failure of bolted containers.[2]</td></tr>
<tr><td>9/28/2165</td><td>2165.743</td><td>178.740</td><td colspan="2">End of institutional control.
Installation of final closure cap.</td></tr>
<tr><td>1/1/2737</td><td>2737.003</td><td>750.000</td><td>Hydraulic failure of steel casks, start of metal corrosion and release.[2]</td><td></td></tr>
<tr><td>9/28/2747</td><td>2747.743</td><td>760.740</td><td></td><td>Hydraulic failure of steel casks, start of metal corrosion and release.[2]</td></tr>
<tr><td>9/28/3165</td><td>3165.743</td><td>1178.740</td><td colspan="2">End of 1,000-year period of performance.</td></tr>
<tr><td>9/28/12165</td><td>12165.743</td><td>10178.740</td><td colspan="2">End of 10,000-year modeling period.[3]</td></tr>
</table>

[1]Conservatively, it is assumed that all the waste at each disposal site is placed at the start of operation.
[2]An alternative scenario is to assume that hydraulic failure of bolted containers occurs 750 years after disposal, simultaneous with the failure of the steel casks, rather than when soil is mounded over the disposal site.
[3]In some cases, modeling may be extended to capture peak fluxes. For example, modeling of Pu-239 and its decay products was extended to 150,000 years to obtain the results shown in Section 4 of this report.

2.4 NRCDA Infiltration

Prior to interim closure at the end of ELLWF operations, infiltration through the NRCDA disposal sites is assumed to be 15.78 in/yr, representative of local conditions in E-Area (flat terrain with little to no vegetation). Following the end of ELLWF operations, it is assumed that an institutional control period of 100 years will ensue. During this period, an interim closure cap will be placed over E-Area waste disposal sites and maintained. Infiltration through the interim closure cap is assumed to be 0.1 in/yr.

Following the end of institutional control, a final closure cap will be placed over all E-Area waste disposal sites without further maintenance. Infiltration through the final closure cap over the NRCDA disposal sites has been calculated separately using the Hydrologic Evaluation of Landfill Performance (HELP) model (Dyer, 2019). Results from the HELP modeling are used as input to the GoldSim model. Table 2.4.1 provides the nominal calculated infiltration rates through the final closure cap over time. Without maintenance, performance of the closure cap slowly degrades, and infiltration approaches a value slightly less than the mean General Separation Area (GSA) infiltration (Flach, 2019) because of transpiration from the assumed vegetation coverage.

The GoldSim model uses Table 2.4.1 for infiltration at NRCDA sites starting at 178.74 years into the simulation (see Table 2.3.1 above). GoldSim uses linear interpolation to calculate infiltration rates at simulation times between those listed in Table 2.4.1.

Table 2.4.1 NRCDA Infiltration with Final Closure Cap in Place

Years from Final Closure Cap Placement	Intact Infiltration Rate (in/yr)
0	0.0008
80	0.007
190	0.16
200	0.18
240	0.30
280	0.38
380	1.39
560	3.23
1000	6.82
1800	10.24
2623	11.10
3200	11.18
5600	11.30
10000	11.35
15000	11.35
150000	11.35

3.0 GoldSim Model Description

The two NRCDA sites (643-7E and 643-26E) are located a significant distance apart. The sites have different footprints, disposal histories, and vadose zone hydro-stratigraphic layers. Despite these differences, it was desirable to have a single GoldSim model that could be used for either site by simply entering different model parameters through model input. The model also needs to include radionuclide releases from either bolted containers or welded steel casks. Bolted containers are assumed to fail instantaneously and release all their waste inventory at once. Container failure is assumed to occur either at the time soil is mounded over the disposal area or 750 years after disposal roughly corresponding to hydraulic failure of welded casks due to weld corrosion (Hang and Hamm, 2019). Welded steel casks are assumed to contain active metal waste that slowly releases radionuclides through metal corrosion. Corrosion and release are assumed to begin 750 years after disposal when the cask itself has corroded and lost hydraulic integrity (Hang and Hamm, 2019).

3.1 Dashboard User Interface

Figure 3.1.1 shows the initial appearance of the GoldSim model dashboard where the user enters values that control the disposal scenario. Using dashboard entries allows changing model parameters without editing the model. Selecting 643-26E or 643-7E as the disposal site by checking the appropriate box at the top of the dashboard specifies the timeline parameters and vadose zone hydro-stratigraphic layers used in the model calculations as described in Sections 2.2 and 2.3.

Figure 3.1.2 shows selection of bolted containers in 643-26E (left-hand-side) or steel casks in 643-7E (right-hand-side). If disposal of bolted containers is selected, checking the box labeled "Soil Cover Release", appearing immediately below the "Bolted Container" check box, specifies that the containers fail when soil is mounded over the waste. If the box is not checked, the containers are assumed to fail 750 years after they are placed at the disposal site. When bolted containers fail, all the waste inventory is immediately released into the soil backfill surrounding the containers (waste zone). Selecting bolted containers also opens a user input box labeled "Container Stacking" where the number of container layers is entered. The box accepts entries of 1, 2 or 3. If the disposal of steel casks is selected, the box below this selection labeled "Inconel Fraction in Metal" is used to specify the fraction of activated waste embedded in Inconel. The remaining metal is assumed to be Zircaloy.

Figure 3.1.1 GoldSim NRCDA model dashboard.

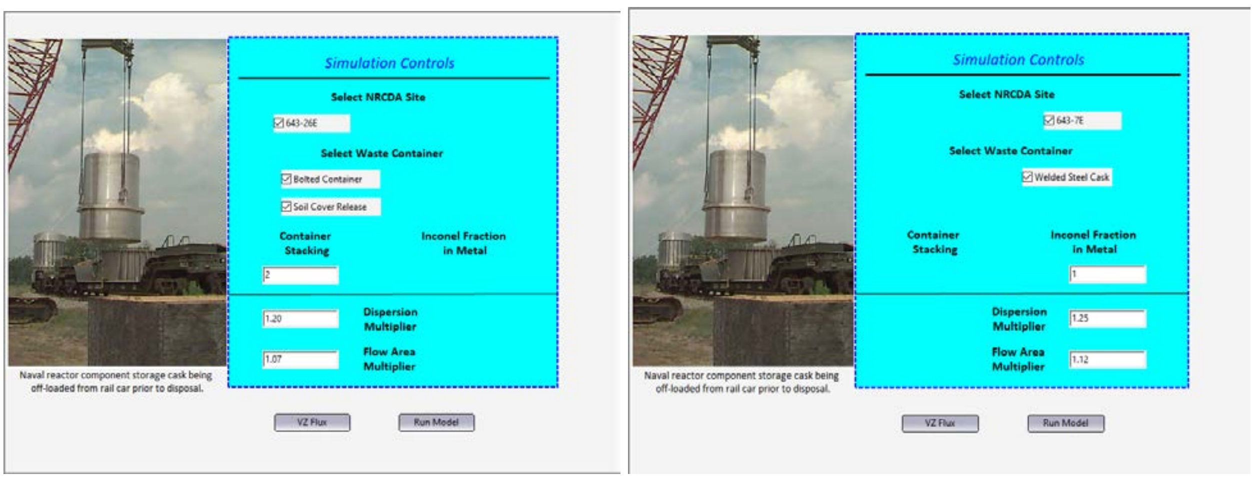

Figure 3.1.2 GoldSim NRCDA model dashboard with bolted containers in 643-26E selected (left) and stainless steel casks in 643-7E selected (right).

The other user input in the lower section of the dashboard, “Dispersion Multiplier” and “Flow Area Multiplier”, give the user limited options to adjust model results. For example, increasing (or decreasing) the contaminant dispersion coefficient in the vadose zone can be used to spread (or sharpen) the contaminant plume and alter the peak concentration to better match PORFLOW results. Similarly, decreasing (or increasing) the effective flow area in the waste and vadose zone could be used to increase (or decrease) the contaminant flow rate to better match PORFLOW results. Water flow into the waste material is calculated as the product of the infiltration rate in Table 2.4.1 and the NRCDA area in Table 2.1.1. The flow area multiplier adjusts flow areas in the waste and vadose zone (nominally the NRCDA area) but does not change the rate of water inflow.

Once dashboard input selections have been made to define the model scenario, the user simply runs the GoldSim model. Results in the form of time histories of radionuclide fluxes to the water table in Ci/yr and mol/yr are collected within GoldSim. These results are easily copied and transferred to Excel for comparison to PORFLOW results. For model benchmarking, active radionuclide species in GoldSim were limited to the short list given in Section 4 of this report. The active species list will be expanded for PA calculations based on final radionuclide screening results and automated output of time history statistics to Excel used to facilitate the uncertainty analysis.

3.2 Materials

Figure 3.2.1 shows the contents of the GoldSim Materials container (yellow box icon) where physical properties for the soil materials are defined. The GoldSim containers with properties for saturated sandy and saturated clayey soil, shown in Figure 3.2.1, will be used to model transport in the aquifer zone below the water table and have no impact on the results presented in this report. Close-compacted backfill (CCBackfill), which describes soil surrounding the waste, was also not used in the model but was retained in the property definitions.

The only unique aspect of the material properties is defining a *Clayey_or_SandySoil* solid material. As is partially shown by the insert to the right of the container picture, the properties are defined using "if" statements that select the property depending on the NRCDA site modeled. For example, the full definition for soil porosity is:

If (Model_26E Then Porosity_ClayeySoil Else Porosity_SandySoil)

The *Clayey_or_SandySoil* material is used in the third vadose zone hydro-stratigraphic layer (i.e. TCZ, see Figure 2.2.1) that contains clayey soil when NRCDA site 643-26E is modeled and sandy soil for NRCDA site 643-7E.

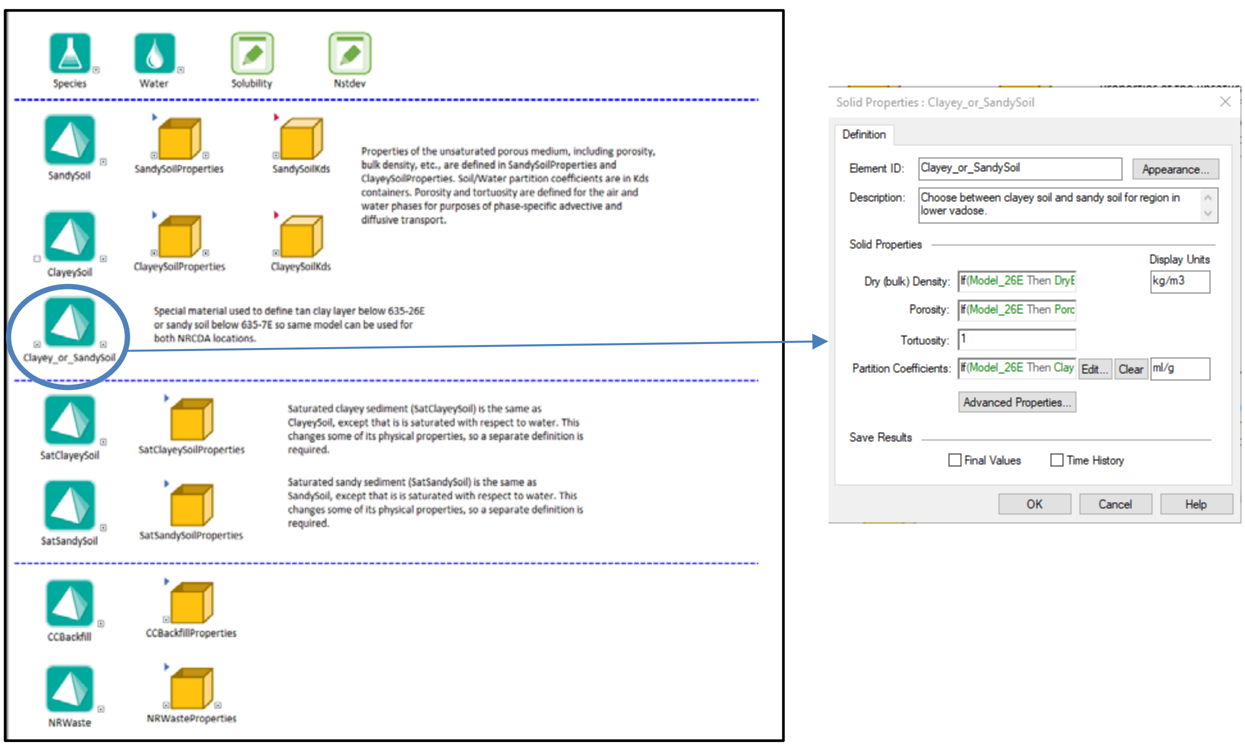

Figure 3.2.1 Contents of materials container where model material properties are defined and detail of *Clayey_or_SandySoil* material definition.

Table 3.2.1 lists nominal values for the soil and waste material properties used in GoldSim vadose zone modeling obtained from Nichols and Butcher (2020). Water content is the product of porosity and saturation.

Table 3.2.1 Soil physical properties used in GoldSim NRCDA model.

Physical Property	Sandy Soil	Clayey Soil	Blended NR Waste
Particle Density (g/ml)	2.67	2.69	2.65
Porosity	0.380	0.385	0.893
Water Saturation	0.912	0.994	0.0927
Water Content (ml/ml)	0.347	0.383	0.0828

3.3 Modeling Radionuclide Decay and Metal Corrosion in Waste

Figure 3.3.1 shows the section of the GoldSim model that calculates radionuclide decay and metal corrosion in the NRCDA waste and release from containment. This section also contains some of the modeling data selected through dashboard input that specify: 643-26E or 643-7E, steel cask or bolted container, fraction of Inconel in activated metal, and early release from bolted containers at time of soil cover or at 750 years. The dashboard input is used to calculate the waste area, waste zone thickness, radionuclide inventory release time, and corrosion rate. The *Initial_Inventory* data is a vector of radionuclide species available for modeling where species to be modeled are given an inventory of 1.0 Ci while species not modeled have zero inventory. At the time of waste disposal, the GoldSim function *SourceInventory* is changed from a species vector of zero inventories to the *Initial_Inventory* vector.

3.3.1 Releases from Bolted Containers

Releases from bolted containers are assumed to occur instantaneously either when the soil cover is placed over the disposal site or 750 years after disposal. The waste simply needs to be confined between the time of disposal at the NRCDA site and the time of release to account for parent decay and daughter ingrowth. This function occurs in cell *BC_Source*. The radionuclide inventory in the cell is set to *SourceInventory*, which, as explained above, will become the set inventory at the time of waste disposal. At the time of release, the one-time event *BC_Waste_Transfer* is set to occur which transfers the decayed waste to the *Waste* aquifer pathway (see Figure 3.4.1).

3.3.2 Releases from Welded Steel Casks

Releases from welded steel casks that depend on corrosion of activated metal holding the radionuclides are more difficult to model. As with bolted containers, between the time of waste disposal and hydraulic failure of the cask (assumed to occur at 750 years) the waste must be confined to account for parent decay and daughter ingrowth. It is further assumed that corrosion of the activated metal does not begin until the cask fails hydraulically. After hydraulic failure, radionuclides are released from the activated metal at the corrosion rate until the metal is depleted. Because much of the activated metal consists of thermal shields and metal plates, the corrosion is modeled as a linear process where the metal is depleted at a constant rate.

The behavior described in the preceding paragraph is modeled in GoldSim as follows. At the time of disposal, the waste inventory is placed into the *Cask_Source* cell where parent decay and daughter ingrowth occur to maintain the correct composition of disposed radionuclides over time. The GoldSim function *CorrosionRate* uses Eq. (1) and Eq. (2) in Section 2.1 to calculate the rate of metal corrosion. Corrosion is assumed to begin at the time of hydraulic failure 750 years after disposal. Corrosion products are transferred to the *Waste* aquifer pathway at the fixed "Input Rate" as shown below in a view of *Waste* aquifer pathway in Figure 3.4.1 of Section 3.4.

Function *Corrosion_Release* calculates the continuous release of corrosion products using the following logic:

1. Release of corrosion products is zero for simulation times less than 750 years or greater than 750 years + 1/*CorrosionRate*, which is the time of complete metal depletion.
2. During the time from 750 years to the time of metal depletion, radionuclides are released at the *CorrosionRate* value having the composition of the decaying metal in cell *Cask_Source*. This is accomplished by creating a continuous input to the *Waste* aquifer pathway. This input stream does not actually transfer material out of *Cask_Source* into *Waste* but simulates a continuous transfer with the correct mass and composition to model linear corrosion of the activated metal.

For the waste inventory in the *Cask_Source* cell, parent decay and daughter ingrowth continue to occur maintaining the correct radionuclide composition over time.

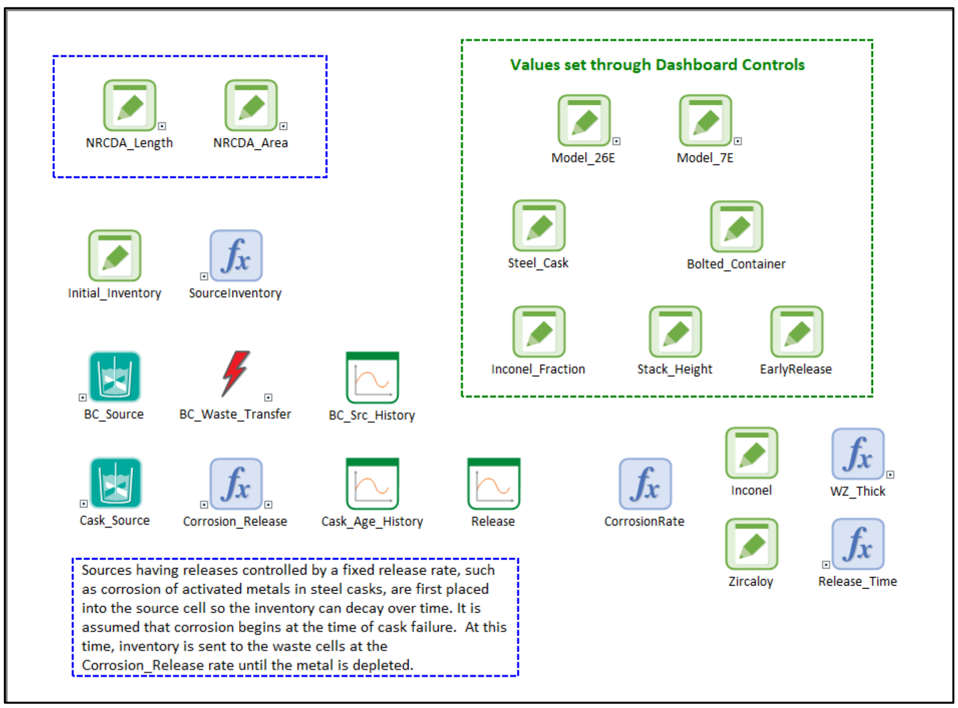

Figure 3.3.1 GoldSim model of radionuclide containment.

3.4 Waste Zone and Vadose Zone Transport Model

Figure 3.4.1 shows the section of the GoldSim model that calculates water flow and radionuclide transport through the waste and vadose zone layers. A connected series of five GoldSim "aquifer pathway" models is used for this purpose. GoldSim aquifer pathway models are a convenient way to create a series of flow cells that are used to model material transport. The insert on the right hand side of Figure 3.4.1 shows the specification of parameters for the *Waste* aquifer pathway model.

Most of the parameters are self-explanatory. The number of cells in the aquifer pathway model is calculated as the aquifer pathway length divided by the nominal cell length of one foot (GoldSim data element *Nom_Cell_Length*) with a minimum of four cells. For example, with a nominal cell length of one foot, the number of cells in each vadose zone aquifer pathway is equal to the segment length shown in Table 2.2.1. In the waste zone, a steel canister would have 18 cells and a single layer of bolted containers four. There are two discrete changes to the *Waste* aquifer pathway inventory from direct transfer events *BC_Waste_Transfer* and *Cask_Waste_Lost* as described in Sections 3.3.1 and 3.3.2 above. Specifying the "*Source Zone Length*" as the waste zone thickness distributes the discrete change inventories and the incoming flow uniformly among the *Waste* aquifer pathway cells.

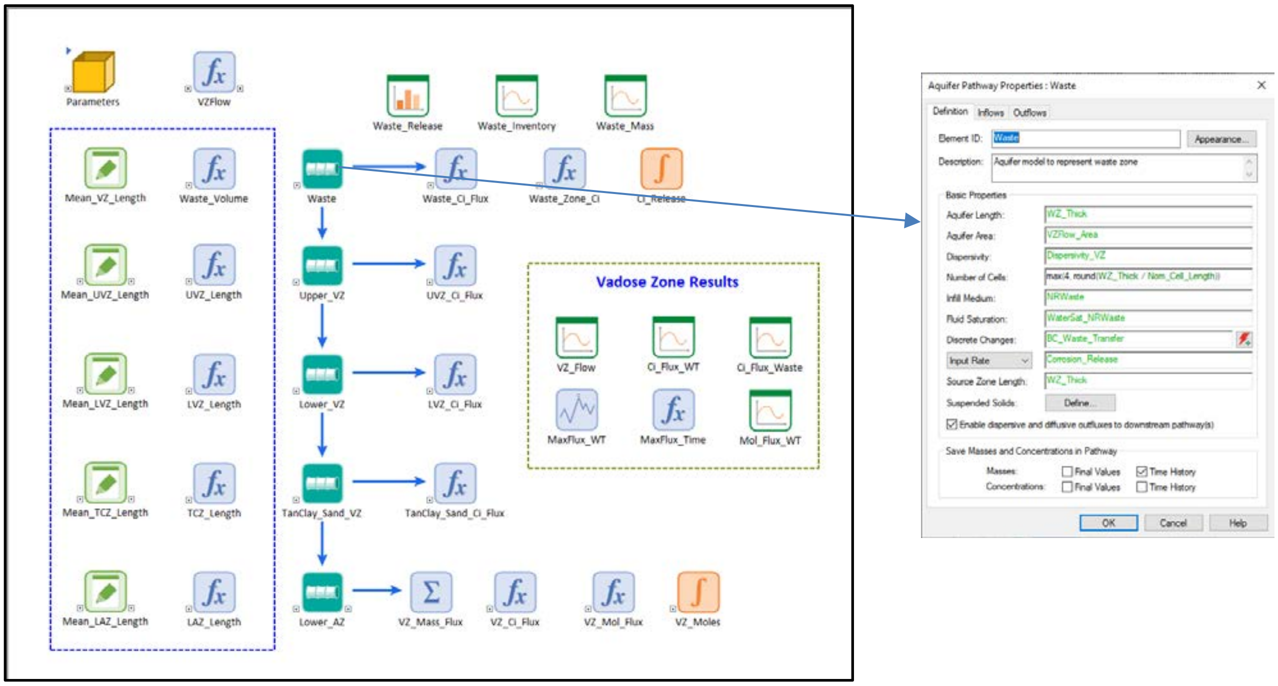

Figure 3.4.1 GoldSim model of transport through waste and vadose zones with detail of *Waste* aquifer model definition.

Calculation of aquifer pathway lengths in the dashed rectangle on the left-hand-side of Figure 3.4.1 will be used for uncertainty analysis to randomly vary the lengths using preassigned distributions. Benchmarking calculations, which are the subject of this report, were all made using the mean (nominal) aquifer lengths given in Table 2.2.1. Figure 3.4.1 shows that fluxes (Ci/yr/Ci buried) are calculated for radionuclides leaving the waste zone and each vadose zone segment. The flux out of the lower aquifer zone is the flux to the water table that was compared to PORFLOW results. The time history of flux to the water table is saved in GoldSim function *Ci_Flux_WT* located in the dashed box labeled "*Vadose Zone Results*" where it can be displayed as either a table of values or a plot. The table can be copied into Excel for further analysis. Maximum fluxes and the times at which they occur are saved in GoldSim functions *MaxFlux_WT* and *MaxFlux_Time*, respectively.

A nominal dispersivity in the vadose zone aquifer models (*Dispersivity_VZ*) was set equal to the nominal cell length of one foot. Dispersivity in GoldSim aquifer pathway cells creates downstream dispersion of cell concentrations. To make this an adjustable parameter that could be used to obtain better comparison with PORFLOW results, a *Dispersion_Factor*, which is a multiplier on the nominal dispersivity, was created and linked to dashboard input as shown in the lower part of Figure 3.1.1. This input allows the user to modify dispersivity in the aquifer pathways through data entry on the dashboard without editing the model. Different factors can be used for the two disposal sites. Similarly, a factor to adjust the flow area at each disposal site was created and linked to dashboard input as seen in Figure 3.1.1. The one-dimensional GoldSim model cannot reproduce two- or three-dimensional flow effects that appear in the PORFLOW models. The simplest adjustments to make are to modify the effective flow area and dispersion.

4.0 Model Benchmarking to PORFLOW

To compare the performance of the GoldSim and PORFLOW models of the NRCDA vadose zone, fluxes to the water table from releases of C-14, I-129, Nb-94, Ni-59, and Tc-99 were evaluated using both models. In addition, to include a decay chain, fluxes to the water table for radionuclides from the release of Pu-239 and its daughters with half-lives greater than one year (Pu-239 → U-235 → Pa-231 → Ac-227) were also evaluated. These radionuclides were chosen as representative of NRCDA waste and significant contributors to the dose. The comparison included release of the radionuclides from double-stacked bolted containers in 643-26E and from carbon steel casks in 643-7E. The calculations all begin with a nominal 1.0 Curie of each parent radionuclide present at the time of disposal. Results from the two scenarios used to benchmark the GoldSim model are described in the following subsections.

4.1 Releases from Bolted Containers in NRCDA 643-26E

The first set of benchmarking comparisons modeled the release of radionuclides from bolted containers at the NRCDA 643-26E site. The release occurs 68 years after disposal, at the start of institutional control, when soil is mounded over the disposal area and containers are assumed to lose hydraulic integrity and release their entire waste inventory. It is assumed that the containers are stacked in two layers with a total height of 8.2 feet. Time zero for the PORFLOW model was set as the start of ELLWF operations. The GoldSim model cannot use negative times; therefore, as shown in Table 2.3.1, the GoldSim model takes time zero to be when the first disposal occurred at the 643-7E site which is 7.74 years earlier. To plot results, GoldSim times were reduced by this 7.74 year offset to correspond with the PORFLOW timing. As can be seen in Figure 3.1.2, the dispersion coefficient used for the 643-26E simulations was 1.20 ft and flow area increased to 1.07 of its nominal value.

Figure 4.1.1 shows a comparison of GoldSim and PORFLOW flux to the water table (Ci/yr/Ci buried) for C-14 and I-129 on linear and log scale plots. Figure 4.1.2 shows a similar comparison for Ni-59 and Tc-99. For these four isotopes, with relatively low solid-liquid distribution coefficients (K_d's), the flux curves from both models are in close agreement with respect to both peak flux and timing although for both C-14 and Ni-59, the GoldSim flux curves elute from the vadose zone slightly sooner. Figure 4.1.3 compares GoldSim and PORFLOW flux to the water table for Nb-94 on linear and log scale plots. In this case, agreement between the peak shape and maximum value in the two models is again good; however, the GoldSim flux curve elutes slightly later.

Figure 4.1.4 shows a linear plot of flux to the water table predicted by both models for Pu-239 and U-235 and a log scale plot of flux to the water table for all members of the Pu-239 decay chain. Figure 4.1.5 shows linear scale plots comparing Pa-231 and Ac-227 flux to the water table from both models. Simulations were run for 150,000 years which was not long enough to capture the peak flux for Pu-239. Results for U-235, Pa-231 and Ac-227 are in very good agreement between the two models. The log plot shows that, as was the case for Nb-94, the GoldSim flux curves for Pu-239 and U-235 initially lag behind the PORFLOW curves at very low flux values. However, the linear plot shows that the GoldSim U-235 peak timing agrees closely with the PORFLOW calculation.

Direct comparisons of peak fluxes and timing of the peaks for release from bolted containers in 643-26E for both models are provided in Table 4.1.1. The largest difference in peak flux is 6% for

Ni-59 with all other peak fluxes within ±4% of each other. The largest difference in timing is 8% for C-14 with the other peak timings agreeing within ±5%.

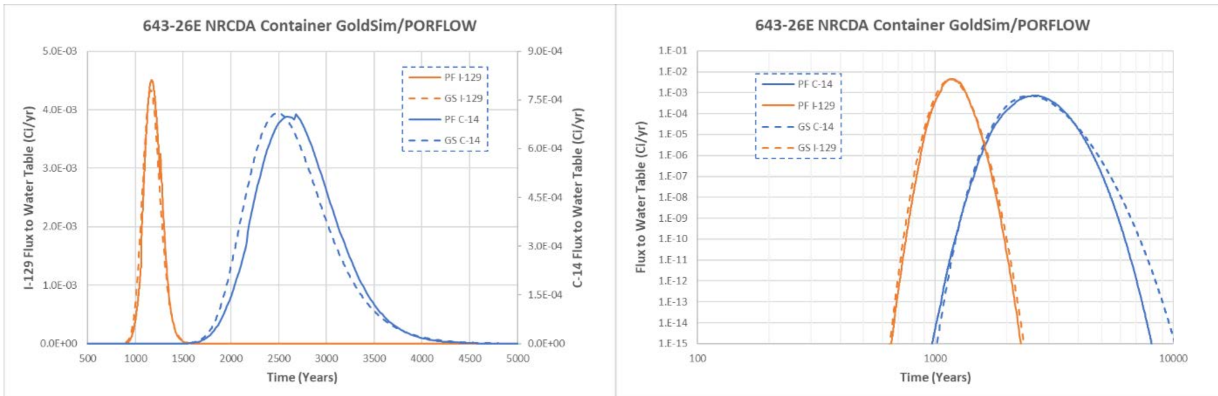

Figure 4.1.1 Linear and log plots of GoldSim and PORFLOW flux to the water table for I-129 and C-14 released from bolted containers in 643-26E.

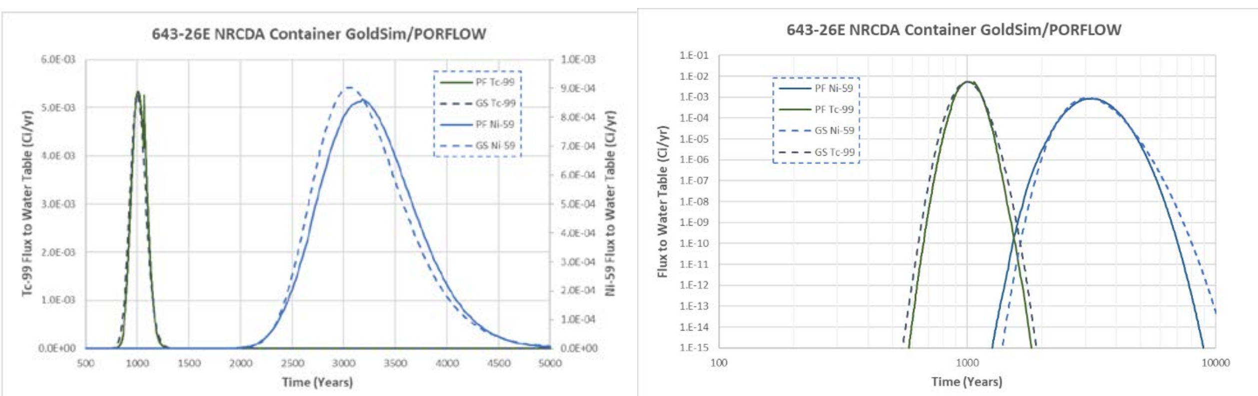

Figure 4.1.2 Linear and log plots of GoldSim and PORFLOW flux to the water table for Tc-99 and Ni-59 released from bolted containers in 643-26E.

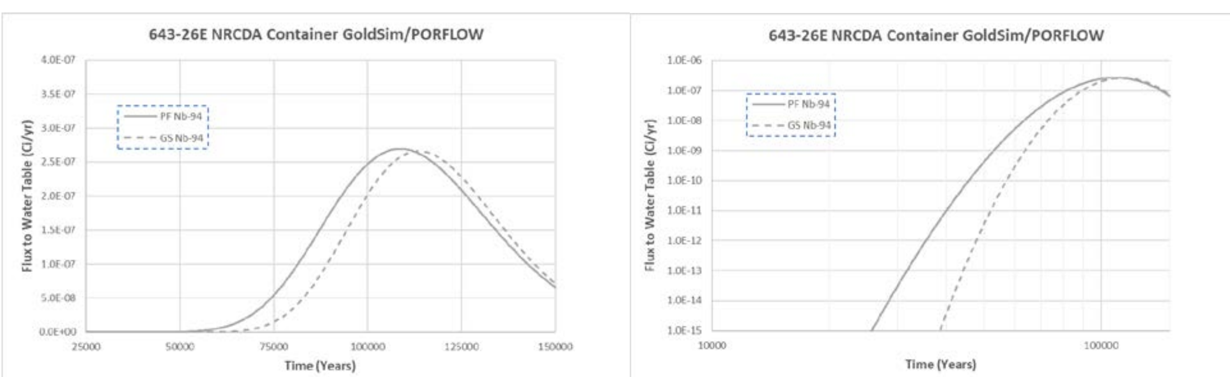

Figure 4.1.3 Linear and log plots of GoldSim and PORFLOW flux to the water table for Nb-94 released from bolted containers in 643-26E.

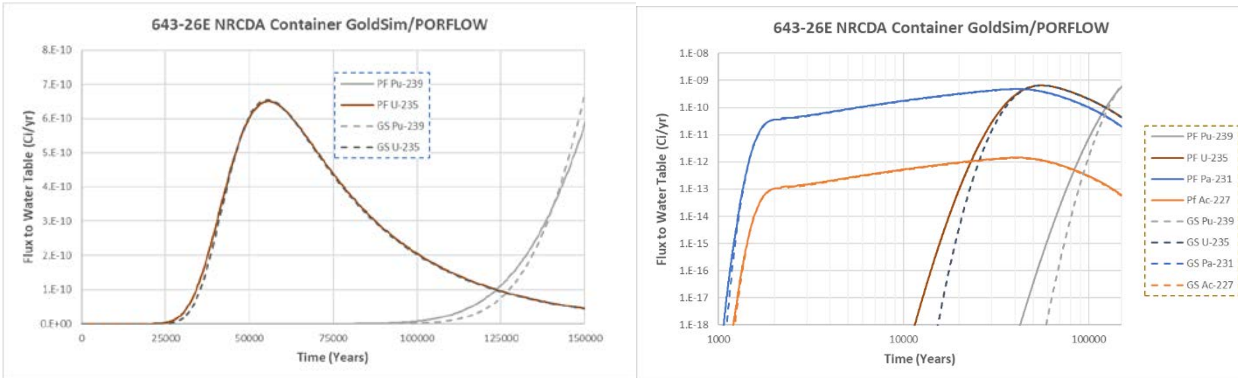

Figure 4.1.4 Linear plot of GoldSim and PORFLOW flux to water table for U-235 and Pu-239 and log plot of fluxes for Pu-239 decay chain nuclides released from bolted containers in 643-26E.

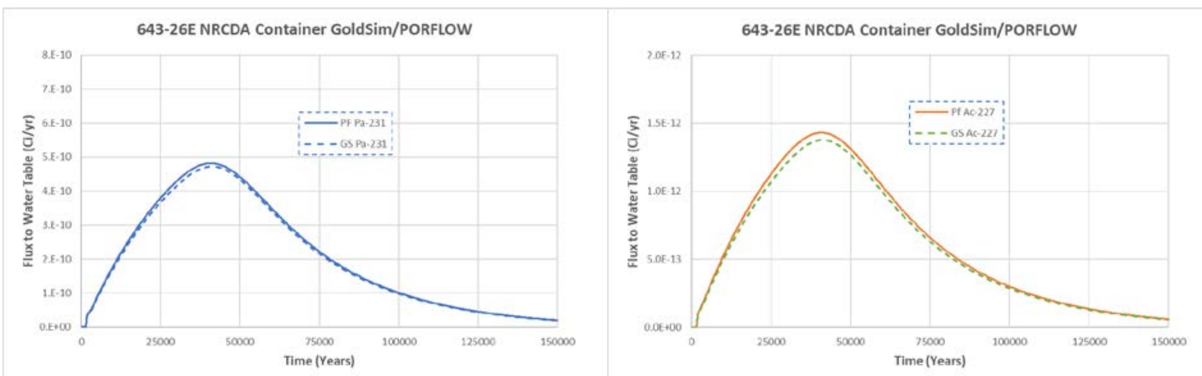

Figure 4.1.5 Linear plots of GoldSim and PORFLOW flux to the water table for Pa-231 and Ac-227 released from bolted containers in 643-26E.

Table 4.1.1 Comparison of GoldSim and PORFLOW peak fluxes to the water table and peak times for releases from bolted containers in 643-26E.

	PORFLOW		GoldSim		Ratio	
	Max Flux	Max Time	Max Flux	Max Time	GoldSim/PORFLOW	
Nuclides	Ci/yr	Year	Ci/yr	Year	Ci/yr	Year
Tc-99	5.337E-03	1007	5.222E-03	990	0.98	0.98
I-129	4.506E-03	1171	4.306E-03	1150	0.96	0.98
C-14	7.067E-04	2683	7.140E-04	2470	1.01	0.92
Ni-59	8.620E-04	3183	9.097E-04	3040	1.06	0.96
Nb-94	2.694E-07	108443	2.644E-07	114050	0.98	1.05
U-235	6.496E-10	55363	6.574E-10	55400	1.01	1.00
Pa-231	4.816E-10	40463	4.732E-10	41180	0.98	1.02
Ac-227	1.431E-12	40263	1.380E-12	40640	0.96	1.01

4.2 Corrosion Release from Welded Steel Casks in NRCDA 643-7E

The second set of benchmarking comparisons modeled the release of radionuclides from welded steel containers located at the NRCDA 643-7E site. In this case, zero time in both models was the time when disposed casks were first placed at the site. The model casks contain radionuclides (1.0 Ci of each parent) embedded in Inconel that are released by metal corrosion. Corrosion is assumed to begin when the casks lose hydraulic integrity 750 years following disposal. As listed in Table 2.1.2, Inconel corrodes at the rate of 6.2194e-05/yr. Therefore, starting at 750 years, this constant amount of the waste inventory is released each year until the metal is fully depleted at 16,079 years. Both models track radioactive decay and ingrowth of daughter products during waste storage and transport following release. As shown in Figure 3.1.2, the dispersion coefficient used for the 643-7E simulations was 1.25 ft and the flow area increased to 1.12 of the nominal value.

Figure 4.2.1 shows a comparison of GoldSim and PORFLOW flux to the water table (Ci/yr/Ci buried) for I-129 and Tc-99 on both linear and log scale plots. Figure 4.2.3 shows a similar comparison of GoldSim and PORFLOW flux to the water table for Ni-59 and C-14. For these four isotopes, the timing of the flux curves and the peak fluxes are within 1% of each other. I-129 and Tc-99 both have small solid-liquid distribution coefficients (K_d's) and long half-lives. Therefore, fluxes for these isotopes start quickly at 750 years followed by steady-state release at the Inconel corrosion rate for about 16,000 years with a rapid termination of the release when the metal is depleted. The small initial surge in flux shown by both models is caused by changes in the infiltration rate. Figure 4.2.2 shows an enlarged view of the initial portion of the flux curves. PORFLOW transport is limited to using discrete flows determined by separate PORFLOW calculations. This creates the “saw tooth” release pattern shown in Figure 4.2.2 as flows change. GoldSim linearly interpolates flow from Table 2.4.1 at each time step which smooths out the flux curve.

Figure 4.2.4 shows log and linear scale plots of Nb-94 flux to the water table calculated using the PORFLOW and GoldSim models. For Nb-94, the GoldSim model predicts a peak flux about 3% lower than the PORFLOW value and a peak time 4% greater. Nb-94 has a half-life of 20,300 years. Additional decay during the 4,180 years difference in peak timing accounts for the lower GoldSim peak value. Figure 4.2.5 shows a linear scale plot comparing flux to the water table for GoldSim and PORFLOW simulations of U-235 and Pa-231 NRCDA vadose zone transport, and a log scale plot of fluxes for all Pu-239 chain nuclides from both models. Figure 4.2.6 shows linear plots of GoldSim and PORFLOW flux to the water table for Ac-227 and Pu-239. As the plots show, model results compare very closely for U-235, Pa-231 and Ac-227. Showing behavior like that seen for Nb-94, the GoldSim Pu-239 flux is significantly lower than the PORFLOW flux over the initial portion of the curve at very small values of the flux.

Direct comparisons of peak fluxes and timing of the peaks for release from welded casks in 643-7E for both models are provided in Table 4.2.1. The largest difference in peak flux is 3% for Nb-94 while the other peak fluxes agree within ±2% of each other. The largest difference in timing is 6% for I-129 with the other peak timings agreeing within ±4%. Careful examination of Figure 4.2.2 finds that the PORFLOW I-129 peak occurs at the first “saw tooth” which may explain the relatively large difference in reported peak times.

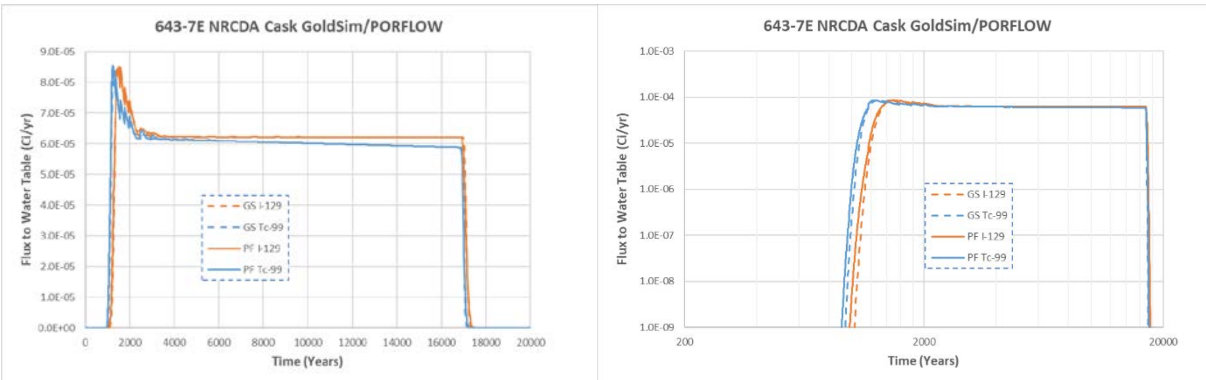

Figure 4.2.1 Linear and log plots of GoldSim and PORFLOW flux to the water table for I-129 and Tc-99 released by Inconel corrosion from steel casks in 643-7E.

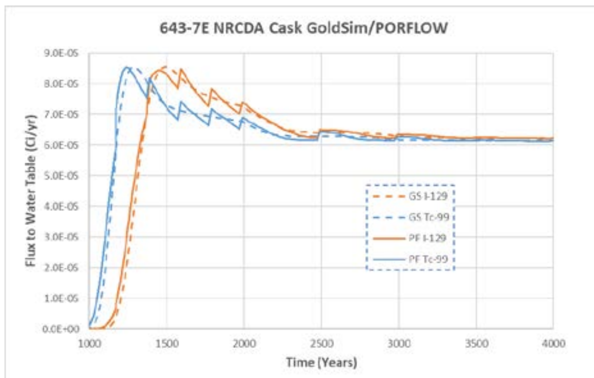

Figure 4.2.2 Expanded view of early GoldSim and PORFLOW flux to the water table for releases of I-129 and Tc-99 by Inconel corrosion from steel casks in 643-7E.

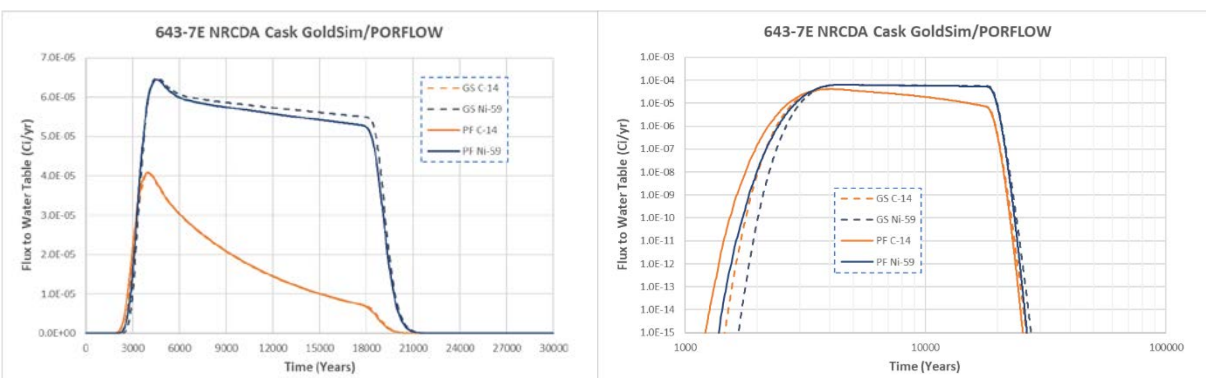

Figure 4.2.3 Linear and log plots of GoldSim and PORFLOW flux to the water table for C-14 and Ni-59 released by Inconel corrosion from steel casks in 643-7E.

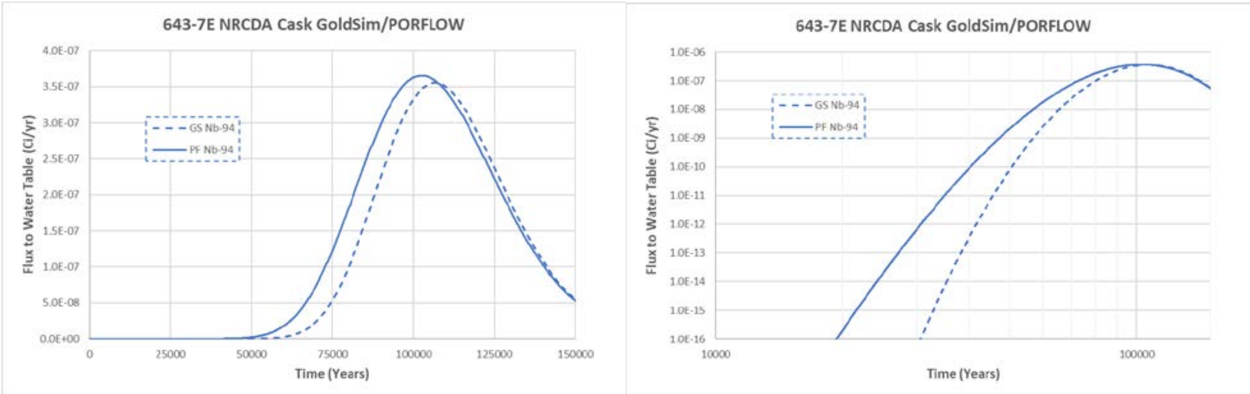

Figure 4.2.4 Linear and log plots of GoldSim and PORFLOW flux to the water table for Nb-94 released by Inconel corrosion from steel casks in 643-7E.

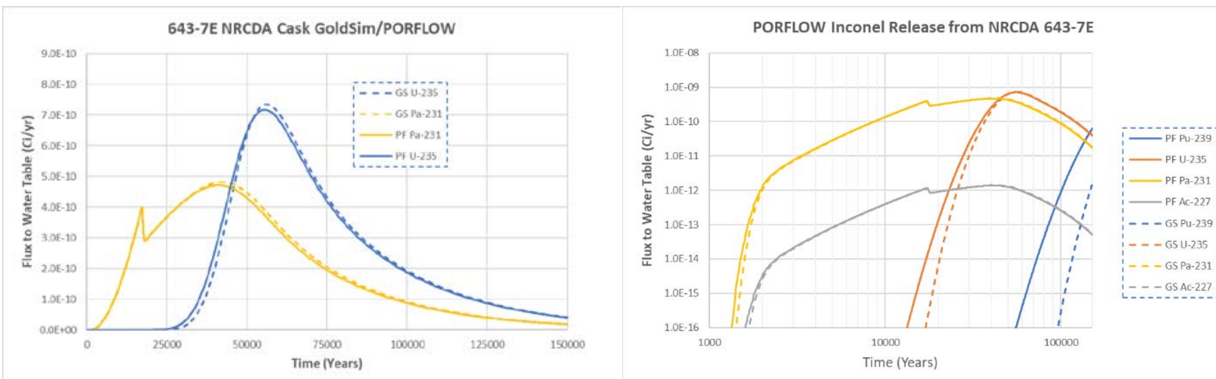

Figure 4.2.5 Linear plot of U-235 and Pa-231and log plot of Pu-239 chain for GoldSim and PORFLOW flux to the water table by Inconel corrosion from steel casks in 643-7E.

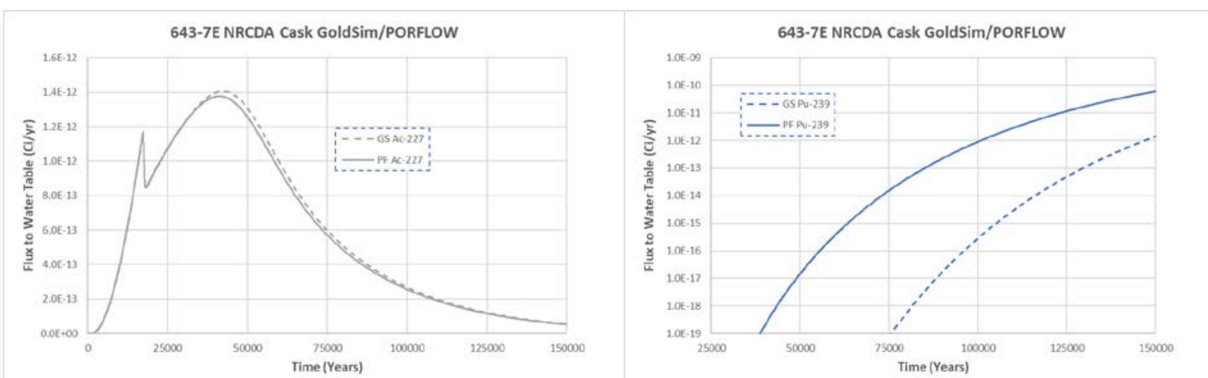

Figure 4.2.6 Linear plot of Ac-227 and semi-log plot of Pu-239 for GoldSim and PORFLOW flux to the water table released by Inconel corrosion from steel casks in 643-7E.

Table 4.2.1 Comparison of GoldSim and PORFLOW peak fluxes to the water table and peak times for releases by Inconel corrosion from steel casks in 643-7E.

Nuclides	PORFLOW		GoldSim		Ratio	
	Max Flux	Max Time	Max Flux	Max Time	GoldSim/PORFLOW	
	Ci/yr	Year	Ci/yr	Year	Ci/yr	Year
Tc-99	8.536E-05	1242	8.532E-05	1285	1.00	1.03
I-129	8.495E-05	1591	8.531E-05	1490	1.00	0.94
C-14	4.086E-05	3991	4.049E-05	4010	0.99	1.00
Ni-59	6.448E-05	4511	6.488E-05	4550	1.01	1.01
Nb-94	3.653E-07	102171	3.552E-07	106350	0.97	1.04
U-235	7.176E-10	55571	7.342E-10	56000	1.02	1.01
Pa-231	4.716E-10	41171	4.816E-10	41940	1.02	1.02
Ac-227	1.377E-12	41171	1.405E-12	41800	1.02	1.02

5.0 Conclusions

A one-dimensional GoldSim model has been developed to calculate the release of radionuclides from waste disposed at the NRCDA sites and transport through the waste burial region and underlying vadose zone. The model calculates flux (Ci/yr/Ci buried) to the water table for parent and daughter radionuclides accounting for radionuclide decay and daughter ingrowth during waste storage and transport. To demonstrate that the GoldSim model provides an accurate representation of radionuclide releases and transport, results from deterministic (best estimate) model calculations were compared to those obtained using a three-dimensional PORFLOW model of the NRCDA vadose zone (Hang and Hamm, 2019). Two cases were run: 1) Instantaneous release of radionuclides from waste canisters buried in 643-26E at the start of institutional control and 2) Release of radionuclides at a constant rate by corrosion of activated metal from steel casks buried in 643-7E starting 750 years after burial. Complete results from this code-to-code benchmarking are provided in Section 4 of this report. GoldSim model results were found to be comparable to those obtained by PORFLOW.

The GoldSim results were obtained by adjusting flow dispersion and flow area from their nominal model settings as shown in Table 5.1 below. The GoldSim cell length of one foot was chosen as the nominal dispersion distance and nominal flow areas are the NRCDA site areas listed in Table 2.1.1. Different adjustment factors were applied for the separate disposal sites. Ideally it would be better if no adjustable parameters were required to "tune" GoldSim results to match PORFLOW. For the 643-26E results in particular, "tuning" became a tradeoff between matching C-14, Ni-59 and Nb-94. As shown in Figure 4.1.1 and 4.1.2, C-14 and Ni-59 elute faster in the GoldSim model than in PORFLOW while, as shown in Figure 4.1.3 Nb-94 elutes later in GoldSim. This behavior made it difficult to adjust GoldSim results to match PORFLOW for all three radionuclides. The fact that flow area needed to be increased to improve model comparisons at both sites indicates that water flow in the PORFLOW vadose zone was somewhat lower than the infiltration rate. Typically, it is difficult to reproduce three-dimensional flow effects with a one-dimensional model and, in that respect, results of this benchmarking study are very good.

Table 5.1 Adjustment Factors Used in GoldSim Model

Disposal Site	Flow Dispersion	Flow Area Multiplier
643-26E	1.20	1.07
643-7E	1.25	1.12

The GoldSim model is intended to be used for Monte Carlo analysis to determine uncertainty in radionuclide concentrations at PA points of assessment. To accomplish this, the vadose zone transport model will be extended to include transport through the aquifer from the NRCDA sites to the E-Area site boundary. A basic model of aquifer transport has been included in the GoldSim model. Aquifer transport calculations will be benchmarked to PORFLOW in a manner similar to that described in this report for vadose zone transport. Some GoldSim parameters have already been input as probability distributions with the nominal values used for all calculations described in this report. These distributions will likely be revised and extended for the PA stochastic analysis. On a high-end work-station, the GoldSim model takes approximately 40 seconds to perform each of the two model calculations described in Section 4.0 running all radionuclides in a single calculation. This short run time makes using the GoldSim model the only practicable way of performing stochastic analysis.

6.0 References

Bagwell, L.A., and P.L. Bennett, 2017, *Elevation of Water Table and Various Stratigraphic Surfaces Beneath E-Area Low Level Waste Disposal Facility*, SRNL-STI-2017-00301, Revision 1, November 2017.

Dyer, J. A., 2019. *Infiltration Data Package for the E-Area Low-Level Waste Facility Performance Assessment*, SRNL-STI-2019-00363, Revision 0. November 2019.

Flach, G. P., 2019. *Updated Groundwater Flow Simulations of the Savannah River Site General Separations Area*, SRNL-STI-2018-00643, Revision 0. January 15, 2019.

GoldSim Technology Group, 2018, *GoldSim Version 12.1, Contaminant Transport Module Version 7.1*, June 2018.

Hamm, L. L., 2019. Technical memorandum, "Confirmation of Disposal Unit Footprints for Use in E-Area Performance Assessment Revision", SRNL-STI-2019-00205, Revision 0, April 12, 2019.

Hang, T. and L.L. Hamm, 2019, *PORFLOW Implementation of Vadose Zone Conceptual Model for Naval Reactor Component Disposal Area in the E-Area Low Level Waste Facility Performance Assessment*, SRNL-STI-2019-00357, Revision 0, September 2019.

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

Wohlwend, J.L. and B.T. Butcher, 2018. *Proposed NRCDA Groundwater Pathway Conceptual Model*, SRNL-STI-2018-00633, Rev. 0, November 2018.

Wilhite, E. L., and G. P. Flach, 2004. *Evaluation of Proposed New LLW Disposal Activity: In-Place Disposal of Naval Reactor Components at the 643-7E Naval Reactor Component Storage Area*, WSRC-RP-2004-00443, Revision 0, June 29, 2004.

WSRC, 2008, *E-Area Low-Level Waste Facility DOE 435.1 Performance Assessment, Chapter 5 Naval Reactor Component Disposal Area*, WSRC-STI-2007-00306, Rev. 0, July 2008.

Yu, A.D., L.M. McDowell-Boyer, J.R. Cook, and K.E. Young, 2002, *Special Analysis: Naval Reactor Waste Disposal Pad (U)*, WSRC-RP-2001-00948, Rev. 2, December 2002.

Distribution:

cj.bannochie@srnl.doe.gov
alex.cozzi@srnl.doe.gov
david.crowley@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
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
ira.stewart@srs.gov
tad.whiteside@srnl.doe.gov
jennifer.wohlwend@srnl.doe.gov