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

Benchmarking Exercises to Validate the Updated ELLWF GoldSim Slit Trench Model

G. A. Taylor

R. A. Hiergesell

November 2013

SRNL-STI-2010-00737, Revision 1

DISCLAIMER

Printed in the United States of America

Prepared for
U.S. Department of Energy

SRNL-STI-2010-00737
Revision 1

Keywords: *Sensitivity, Uncertainty, Performance Assessment*

Retention: *Permanent*

Benchmarking Exercises to Validate the Updated ELLWF GoldSim Trench Models

G. A. Taylor

R. A. Hiergesell

November 2013

Savannah River National Laboratory™

OPERATED BY SAVANNAH RIVER NUCLEAR SOLUTIONS

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

REVIEWS AND APPROVALS

AUTHORS:

____

G. A. Taylor, Radiological Performance Assessment Date

____

R. A. Hiergesell, Radiological Performance Assessment Date

TECHNICAL REVIEW:

____

K. M. Catlett, Neptune and Company[a] Date

____

B. T. Butcher, Radiological Performance Assessment Date

APPROVAL:

____

D. A. Crowley, Manager Date
Radiological Performance Assessment

____

R. S. Aylward, Manager Date
Environmental Restoration Technology

[a] Neptune and Company (Catlett) reviewed Revision 0 and authorized SRNL to sign for their review. No changes were made to the analysis or results between Revision 0 and Revision 1.

EXECUTIVE SUMMARY

The Savannah River National Laboratory (SRNL) results of the 2008 Performance Assessment (PA) (WSRC, 2008) sensitivity/uncertainty analyses conducted for the trenches located in the E-Area LowLevel Waste Facility (ELLWF) were subject to review by the United States Department of Energy (U.S. DOE) Low-Level Waste Disposal Facility Federal Review Group (LFRG) (LFRG, 2008). LFRG comments were generally approving of the use of probabilistic modeling in GoldSim to support the quantitative sensitivity analysis. A recommendation was made, however, that the probabilistic models be revised and updated to bolster their defensibility. SRS committed to addressing those comments and, in response, contracted with Neptune and Company to rewrite the three GoldSim models.

The initial portion of this work, development of Slit Trench (ST), Engineered Trench (ET) and Components-in-Grout (CIG) trench GoldSim models, has been completed. The work described in this report utilizes these revised models to test and evaluate the results against the 2008 PORFLOW model results. This was accomplished by first performing a rigorous code-to-code comparison of the PORFLOW and GoldSim codes and then performing a deterministic comparison of the two-dimensional (2D) unsaturated zone and three-dimensional (3D) saturated zone PORFLOW Slit Trench models against results from the one-dimensional (1D) GoldSim Slit Trench model.

The results of the code-to-code comparison indicate that when the mechanisms of radioactive decay, partitioning of contaminants between solid and fluid, implementation of specific boundary conditions and the imposition of solubility controls were all tested using identical flow fields, that GoldSim and PORFLOW produce nearly identical results. It is also noted that GoldSim has an advantage over PORFLOW in that it simulates all radionuclides simultaneously – thus avoiding a potential problem as demonstrated in the Case Study (see Section 2.6). Hence, it was concluded that the follow-on work using GoldSim to develop 1D equivalent models of the PORFLOW multi-dimensional models was justified.

The comparison of GoldSim 1D equivalent models to PORFLOW multi-dimensional models was made at two locations in the model domains – at the unsaturated-saturated zone interface and at the 100m point of compliance. PORFLOW model results from the 2008 PA were utilized to investigate the comparison. By making iterative adjustments to certain water flux terms in the GoldSim models it was possible to produce contaminant mass fluxes and water concentrations that were highly similar to the PORFLOW model results at the two locations where comparisons were made.

Based on the ability of the GoldSim 1D trench models to produce mass flux and concentration curves that are sufficiently similar to multi-dimensional PORFLOW models for all of the evaluated radionuclides and their progeny, it is concluded that the use of the GoldSim 1D equivalent Slit and Engineered trenches models for further probabilistic sensitivity and uncertainty analysis of ELLWF trench units is justified.

A revision to the original report was undertaken to correct mislabeling on the y-axes of the compliance point concentration graphs, to modify the terminology used to define the “blended” source term Case for the saturated zone to make it consistent with terminology used in the 2008 PA, and to make a more definitive statement regarding the justification of the use of the GoldSim 1D equivalent trench models for follow-on probabilistic sensitivity and uncertainty analysis.

This page is left blank intentionally

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ACRONYMS AND ABBREVIATIONS

ACRI	Analytical and Computational Research, Inc. (PORFLOW developer)
CIG	Components-in-Grout
ELLWF	E-Area Low-Level Waste Facility
ET	Engineered Trench
GoldSim	Monte Carlo Simulation Software
GTG	GoldSim Technologies Group
PA	Performance Assessment
PORFLOW	Porous-Media Flow and Transport FORTRAN code
SP	Service Pack
SRNL	Savannah River National Laboratory
ST	Slit Trench
SZ	Saturated zone
UZ	Unsaturated zone
LFRG	Low-Level Waste Disposal Facility Federal Review Group
SRS	Savannah River Site
SRNL	Savannah River National Laboratory
WSRC	Washington Savannah River Company
U.S. DOE	United States Department of Energy
1D	One dimensional
2D	Two dimensional
3D	Three dimensional
cm	centimeter
cm/yr	centimeter per year
g	gram
g/cm^3	grams per cubic centimeter
g/L	grams per liter
K_d	Sorption or partitioning coefficient
m	meter
mg/L	milligrams per liter
mol/yr	moles per year
Pu	Plutonium
U	Uranium

1.0 Introduction

As part of the 2008 ELLWF PA (WSRC, 2008) different modeling exercises were performed to predict the emanation of disposed radionuclides from the individual disposal facilities such that disposal limits could be prescribed. Although some radionuclides are released into the atmosphere above the facility, the predominant release pathway leading to exposures to any member of the public is via the groundwater pathway, hence PA model development focused on this mode of release. In PA models, the groundwater release pathway was evaluated in a deterministic mode using the commercially available numerical PORFLOW code (ACRI, 2008). In addition to this, and in compliance with DOE Order 435.1 (DOE, 1999), a sensitivity and uncertainty analysis was also conducted. To perform the PA uncertainty analysis, the commercially available GoldSim code (GTG, 2007) was used to develop models of the three types of ELLWF trenches: Slit Trenches, Engineered Trenches and the Component-in-Grout Trenches. Following this, the sensitivity portion of the analysis was conducted using these models in probabilistic mode and post-processing the results to identify the most sensitive parameters in the system.

The results of the PA sensitivity/uncertainty analyses were subject to review by the U.S. DOE LFRG as part of determining the suitability of the ELLWF for continued use for the disposal of radioactive waste at the Savannah River Site (SRS). LFRG comments were approving of the sensitivity/uncertainty analysis and the use of probabilistic modeling in GoldSim to support the quantitative sensitivity analysis. A recommendation was made, however, that the probabilistic models be revised and updated to bolster their defensibility. SRS committed to addressing those comments and, in response, contracted with Neptune and Company to rewrite the three GoldSim models.

Neptune and Company has completed work to produce updated ST, ET and CIG GoldSim models.(Tauxe and Catlett, 2010). The work described in this report utilizes these revised models to test and evaluate the results against the 2008 PORFLOW model results. This was accomplished by first performing a rigorous code-to-code comparison of the PORFLOW and GoldSim codes and then performing a deterministic comparison of the 2D unsaturated zone and 3D saturated zone PORFLOW models against results from the 1D GoldSim ST model. The purpose of this exercise was to establish that the deterministic GoldSim models produce sufficiently similar results to enhance the credibility of the probabilistic analysis using those models.

2.0 Uncertainty Model Development

This section describes the enhancements made to the 2008 PA GoldSim trench models for the ST, ET and CIG trenches (Tauxe and Catlett, 2010). This work built upon the original 2008 PA GoldSim models to produce updated models that could be tested in the benchmarking phase of the investigation and later in the sensitivity/uncertainty phase of the investigation. The current GoldSim platform, version 10.11 Service Pack (SP) 3 (GTG, 2010), was used to implement the new development work. Briefly, the major improvements included:

- A re-structuring of the waste and unsaturated zones to include dual columns so as to enable the simulation of contaminant transport associated with both Crushable and Non-Crushable waste forms in the Slit and Engineered trenches.

- The implementation of a so-called "uniform" SRS species list. This list is a superset of all modeled radioactive and stable radionuclides from the multiple SRS GoldSim models developed within different modeling groups, many of which have different sets of isotopes to simulate.
- The introduction of a Model Chronology module (container) to keep track of time-related events.
- The ability to run GoldSim in "benchmarking" mode so that a detailed comparison with the PA PORFLOW models, as described later in the report, could be made. This mode included the ability to invoke the set of K_d values employed in the 2008 PA.
- The introduction of a number of user interface improvements, or "Dashboards," within which adjustments to key parameters can easily be made between simulations.

This development work was conducted jointly by Neptune and Company, with consultation and guidance from SRNL's Radiological Performance Assessment Group.

2.1 PORFLOW-GoldSim Code-to-Code Benchmarking Analysis

Before benchmarking the updated 1D GoldSim ELLWF model deterministic results against the 2008 PA PORFLOW model results, a code-to-code benchmarking evaluation was performed. The purpose of this exercise was to demonstrate whether or not the two codes implement the contaminant transport mechanisms in a similarly satisfactory manner before moving on to the second phase of this investigation.

The code-to-code comparison evaluated the mechanisms of radioactive decay, contaminant transport retardation via the partitioning coefficient (or K_d) concept, and implementation of solubility limits for constrained solutions. Additionally, a solubility constrained problem was evaluated to demonstrate the potential for errors in establishing disposal facility limits when multiple radionuclides are not simultaneously modeled.

2.2 Modeling Codes

PORFLOW version 6.10.3 (ACRI, 2008) is a comprehensive computer program for simulation of transient or steady-state fluid flow, heat, salinity and mass transport in multi-phase, variably saturated, porous or fractured media with dynamic phase change. The geometry may be 2D or 3D, Cartesian or cylindrical, the porous/fractured media may be anisotropic and heterogeneous, arbitrary sources or sinks (injection or pumping wells) may be present and, chemical reactions or radioactive decay may take place. It accommodates alternative fluid and media property relations and boundary conditions. It is a proprietary code of Analytical and Computational Research, Inc. (ACRI).

GoldSim version 10.11 (SP3) (GTG, 2010) is an analytical contaminant transport code developed by the GoldSim Technology Group (GTG). When the flow field is specified, it has the ability to compute both advective and diffusive transport of contaminant species; however it lacks the ability to compute advective groundwater movement. The code is normally implemented using a 1D arrangement of computational elements to approximate a flow domain although 2D meshes can be configured. Radioactive decay and chemical retardation within a flow field are easily implemented and multiple contaminants can be simulated simultaneously. One of the main functional features of the code is its ability to perform multiple realizations for stochastic analysis and flexibility in selection of probability density functions for uncertain parameters.

2.3 Analysis

The code-to-code comparison, using PORFLOW and GoldSim, evaluated the processes of radioactive decay, contaminant transport retardation via the K_d concept, and implementation of solubility limits for solutions requiring such a constraint. A simple transport model was established such that it could be implemented within both codes, and the results of simulations conducted with identical initial conditions, noding, and time steps could be evaluated. Finally, a case study of a potential pitfall when solubility constraints are factored into the analysis is presented.

The simple Base Case model was a column of 10 computational elements populated with sand. An illustration of this model domain is presented in Figure 2-1. The dimensions of individual computational cells were set to 1m x 1m x 1cm. In this convention, 1m refers to the width and length of the computational cell, while 1cm refers to the unit depth. The overall length of the 10-cell column (stack of 10 cells) was therefore 10m, as illustrated in Figure 2-1. The lateral boundaries of the column were established as no-flow boundaries and one end of the column assigned an influx of 40 cm/yr. A group of contaminant species were introduced at the influx end and the contaminant mass fluxes at the exit end of the column were evaluated. The contaminant species included a tracer (non-radioactive, non-retarded), ^{14}C, ^{3}H, ^{99}Tc, ^{233}U and ^{234}U. PORFLOW simulations evaluated each species individually, allowing ingrowth of daughter radionuclides. GoldSim simulations evaluated all species in a single simulation and also accommodated ingrowth of daughter radionuclides. Saturated conditions were established in both codes.

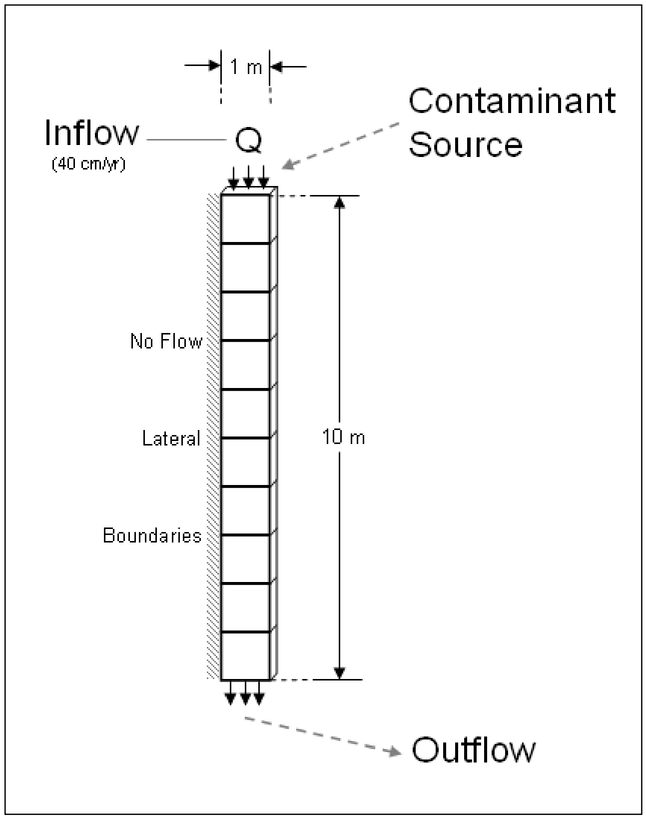

Figure 2-1. 1-Dimensional Flow Domain Implemented within PORFLOW and GoldSim

Materials present within the computational elements included sand and water. The sand was defined as having a porosity of 0.39, a particle density of 2.66 g/cm^3 (or bulk density = 1620 g/cm^3), and diffusivity of 167.25 cm^2/yr. Advective and diffusive transport of contaminants was enabled within both codes. Tortuosity was assumed to be one in both models. A summary of the radionuclides simulated, their half-lives, K_d's and relevant progeny are presented in Table 2-1.

Table 2-1. Contaminant Species Evaluated and Relevant Transport Properties/Information

Isotope	Half Life (yrs)	K_d in Sand (ml/g)	Progeny
^{14}C	5.73E+03	0	
^{3}H	1.23E+01	0	
^{99}Tc	2.11E+05	0.1	
^{233}U	1.59E+05	200	^{229}Th
^{234}U	2.46E+05	200	^{230}Th→^{226}Ra→^{210}Pb
^{229}Th	*7.34E+03*	*900*	
^{230}Th	*7.55E+04*	*900*	*^{226}Ra→^{210}Pb*
^{226}Ra	*1.6E+03*	*5*	*^{210}Pb*
^{210}Pb	*2.22E+01*	*2000*	

Note: Radionuclide species listed in italics were progeny of the parent species. Their presence in the simulation was due strictly to ingrowth

2.4 Results of the Base Case Analysis

The implementation of the transport domain was carefully made to ensure an identical representation in both codes. A failure to achieve identical implementation prevents a meaningful determination of whether the codes are implementing the transport mechanisms appropriately. Ultimately, the ability to produce very nearly identical results is taken as proof that both codes are functioning similarly. Comparisons to analytical solutions of steady-state one and two dimensional flow and contaminant transport problems have been undertaken elsewhere to ensure that both codes are functioning properly (Aleman, 2007). The results for the radionuclides listed in Table 2-1 are presented in Figure 2-2 through Figure 2-6. An examination of these figures reveals that the output from both codes plot in an identical fashion. Such close adherence of the results indicates that the PORFLOW and GoldSim codes are both implementing the contaminant transport mechanisms correctly.

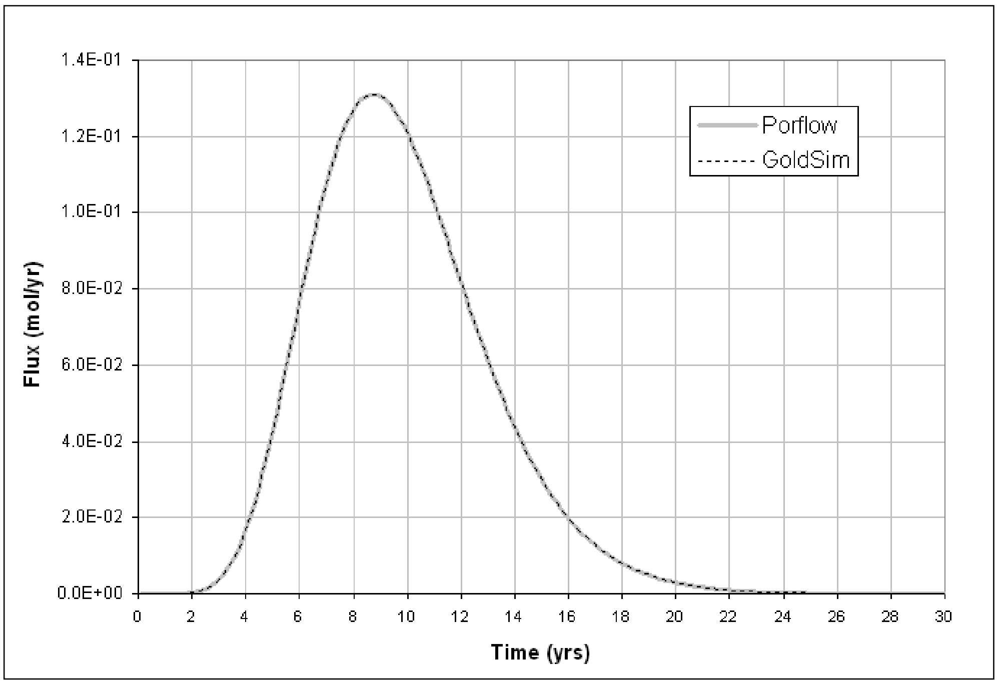

Figure 2-2. ^{14}C breakthrough Curves from the PORFLOW and GoldSim Models

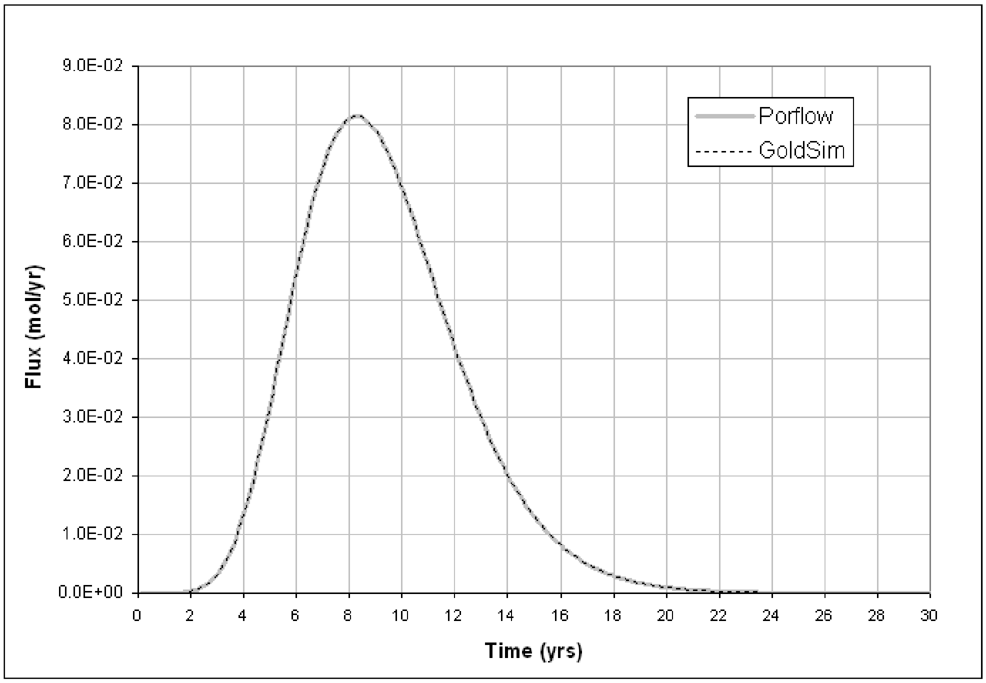

Figure 2-3. ^{3}H breakthrough Curves from the PORFLOW and GoldSim Models

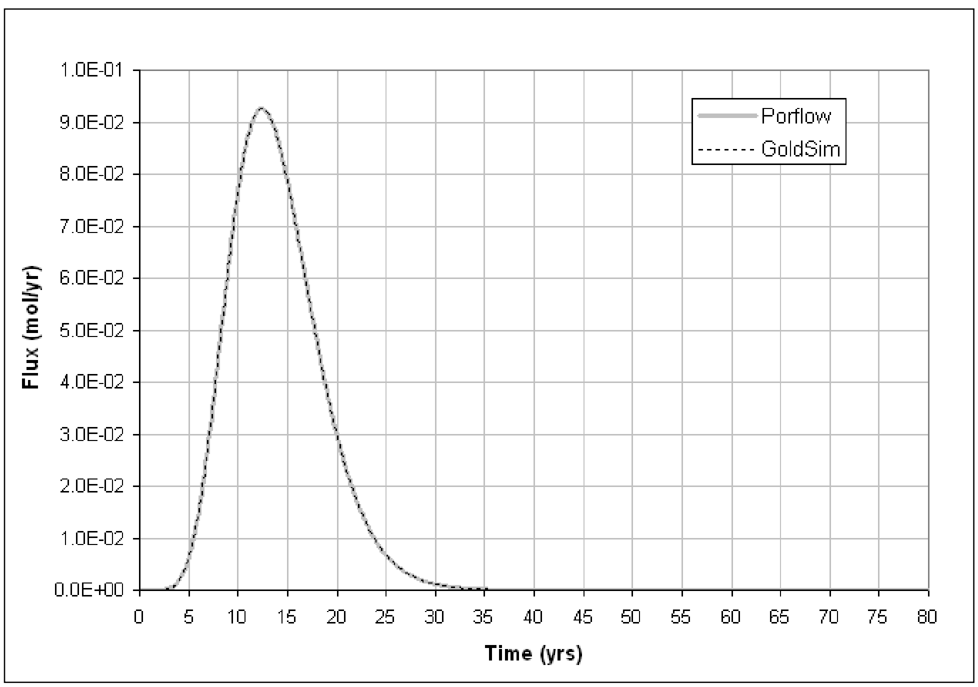

Figure 2-4. ^{99}Tc Breakthrough Curves from the PORFLOW and GoldSim Models

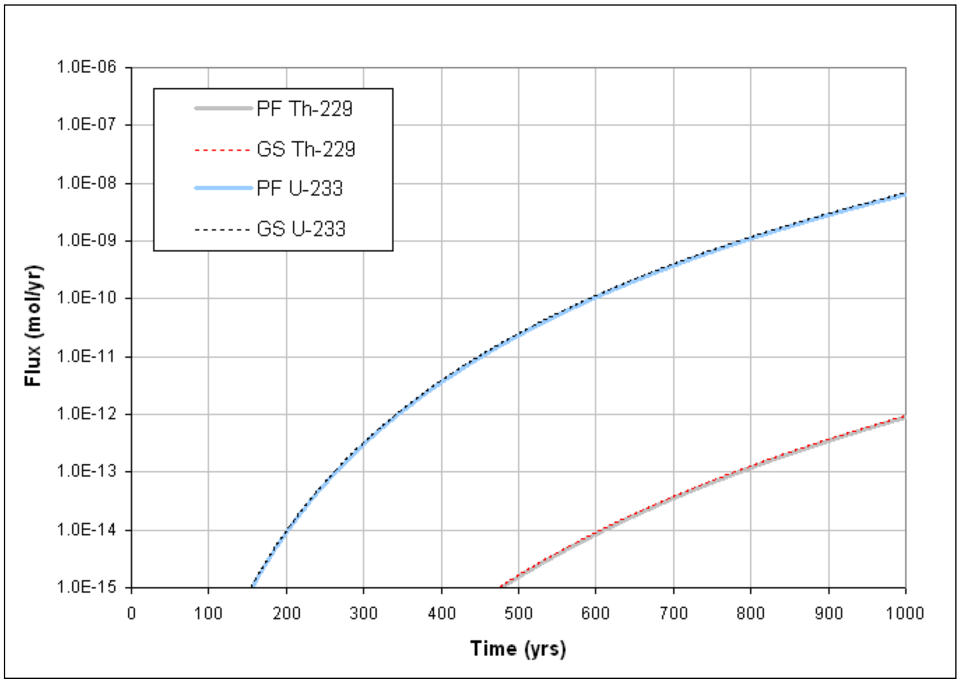

Figure 2-5. ^{233}U and Progeny Breakthrough Curve from PORFLOW and GoldSim Models

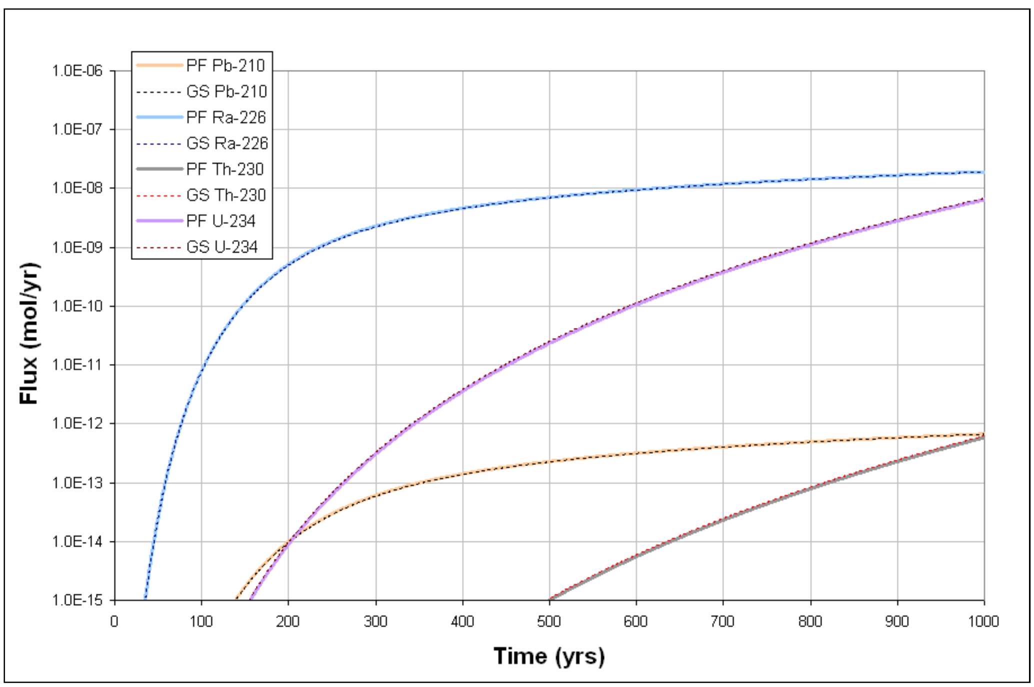

Figure 2-6. ^{234}U and Progeny Breakthrough Curve from PORFLOW and GoldSim Models

2.5 Imposition of a Solubility Limit

Beyond the Base Case comparison, in which the ability to implement radioactive decay and contaminant transport in accordance with the K_d concept, a comparison was made of the ability of PORFLOW and GoldSim to impose a solubility limit. Again, the Base Case model domain, material properties and other assumptions were retained, with the only change being the imposition of the solubility limit. An arbitrary concentration limit for ^{99}Tc of 1200 mg/L was selected and an arbitrarily high source term of 1.0E+06 moles of ^{99}Tc was introduced into the model. The simulation results from both codes produced identical breakthrough curves, approaching the solubility limit at approximately 27 years. The results from both GoldSim and PORFLOW are presented in Figure 2-7. Both results leveling out at the solubility limit indicates that both codes correctly implement the species solubility constraints.

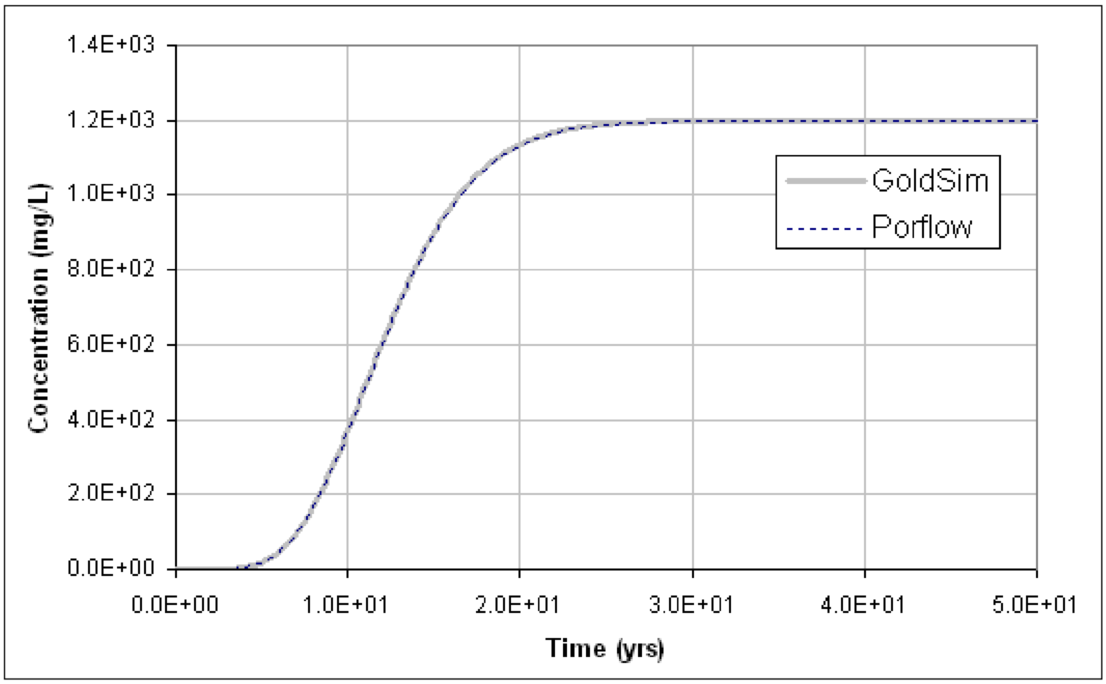

Figure 2-7. Results of Solubility Constrained Solution for ^{99}Tc

2.6 Case Study – Multiple Isotopes of an Element Simulated in a Solubility Constrained Environment

A potential pitfall in SRS PA analyses exists when, as is the normal simulation strategy, the suite of radionuclides simulated to establish disposal limits are simulated individually, in separate PORFLOW simulations. In the situation where a solubility limit for a particular element is an important consideration in these calculations, determining the actual concentration of a particular element in the transport zones can be very difficult if the element has several isotopes that are being simulated separately in the analysis. Additionally, it is not uncommon for one parent radionuclide to decay into one of the other parent radionuclides as it proceeds through its decay chain. The potential exists to overestimate the total elemental concentration within the transport zones if the results of those separate simulations are not combined to determine the actual concentration. An example of this is represented by the different plutonium (Pu) isotopes, each of which decays and produces different uranium (U) isotopes. When an anticipated waste package contains multiple Pu and U isotopes the total mass of either Pu or U present in the system at any time cannot easily be evaluated without carefully summing up the mass of U in the system, at all times, from multiple simulations, as well as keeping track of the residual saturation in order to convert Pu and/or U mass to concentration in pore water. The determination of whether the solubility limit is approached anywhere within the transport zones must be determined external to the main transport code, which is time-consuming and prone to the introduction of errors.

The following hypothetical case was evaluated to illustrate this pitfall. Two uranium isotopes, ^{233}U and ^{234}U were simulated separately as the parent radionuclides within the PORFLOW code using the Base Case model domain and the contaminant transport parameters identified earlier. The ^{233}U source term was set to 100 moles and the ^{234}U source term was set to 10 moles. Each parent was initially simulated without a solubility constraint imposed upon the system and the concentration results of these simulations are illustrated in Figure 2-8. The peak concentration of ^{233}U was 1.82E+04 mg/L and for ^{234}U was 1.82 E+3 mg/L.

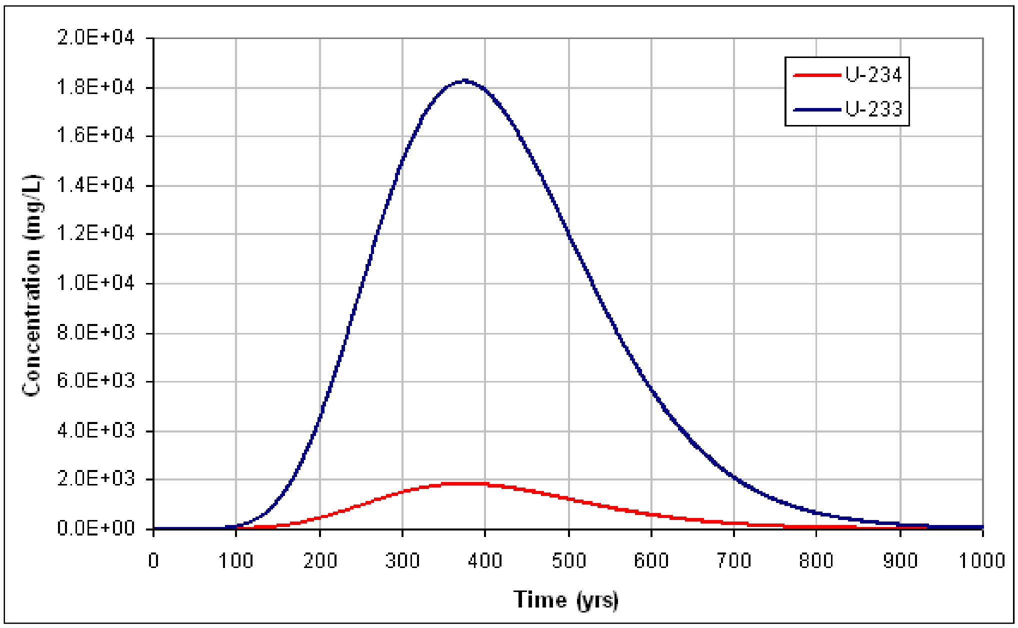

Figure 2-8. ^{233}U and ^{234}U Simulated without Solubility Constraint

Then a parallel simulation was performed using the GoldSim code. All conditions were duplicated except for the fact that both parent isotopes, ^{233}U and ^{234}U, were simulated together, simultaneously within the same model run, taking advantage of GoldSim's ability to simulate multiple species within the same realization. As expected, the GoldSim results were identical to the PORFLOW results for both radionuclides.

Next a solubility constraint was implemented within each model and the simulations repeated. The solubility limit of 6.0E+3 mg/L was selected because it fell between the peak concentrations that were realized for ^{233}U and ^{234}U. The results produced from these PORFLOW and GoldSim simulations were very different and attributable to the fact that PORFLOW simulated ^{233}U and ^{234}U in separate realizations and GoldSim simulated both isotopes together, simultaneously within the same model realization. These results are shown in Figure 2-9.

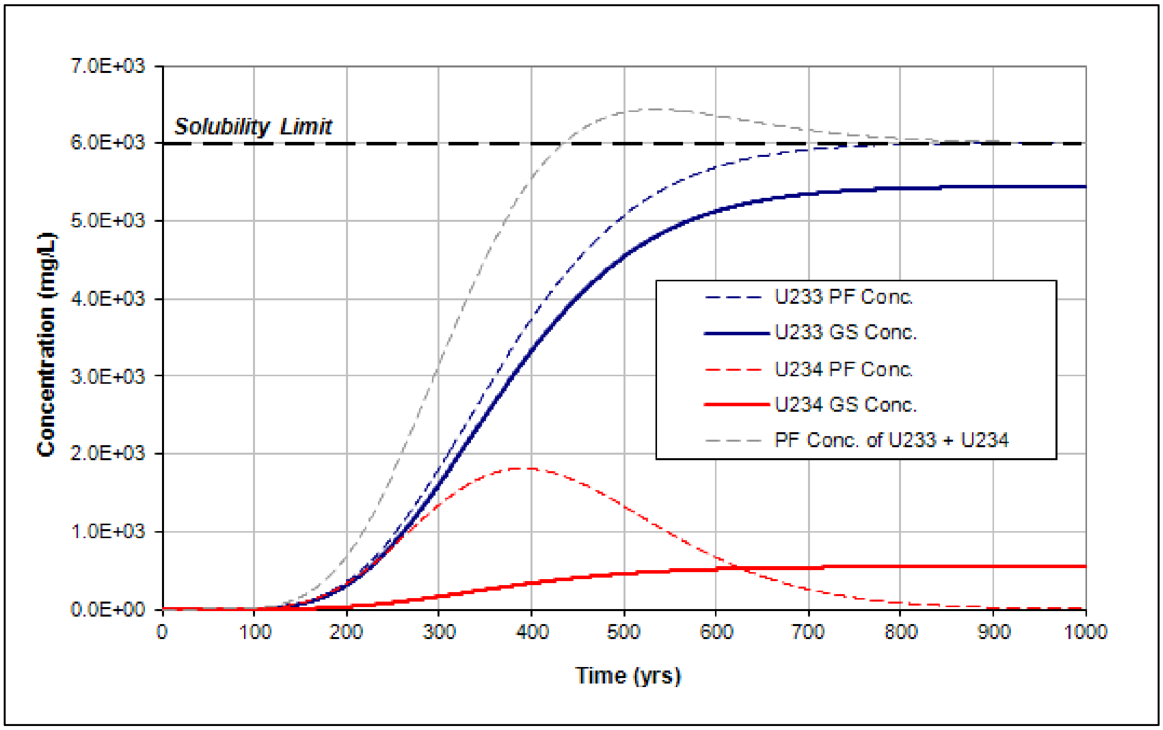

Figure 2-9. ^{233}U and ^{234}U Simulated Individually and Together, with Solubility Constraint

The GoldSim results are illustrated by the solid blue and red lines and are thought to represent the more realistic concentration profiles because they were simulated together. When the sum of the concentrations for both ^{233}U and ^{234}U are tracked through time, the total concentration approaches the solubility limit but never exceed it. Individually, the maximum concentrations for ^{233}U and ^{234}U were calculated to be 5.44E+03 and 5.48E+02 mg/L, respectively.

Results from the separate PORFLOW simulations for ^{233}U and ^{234}U are also shown in Figure 2-9 as the dashed blue and red lines. The simulated concentration profile for ^{233}U approaches the solubility limit while the concentration profile for ^{234}U is identical to the ^{234}U profile realized in the absence of the solubility limit (see Figure 2-8). When the concentrations of ^{233}U and ^{234}U from these separate realizations are summed, the combined concentration profile (dashed gray line) actually exceeds the solubility limit for a period of time. This serves to underscore the point that these results are less realistic than the GoldSim situation, where both isotopes of uranium were simulated together.

A similar situation can occur when a particular parent is simulated within an individual PORFLOW simulation, and a different parent (simulated separately) produces an ingrowth of the former parent radionuclide as it undergoes radioactive decay through time. Such a relationship occurs, for example, with ^{238}Pu and ^{234}U, two radionuclides often found in SRS disposal facility anticipated closure inventories.

The point to be made is that investigators using the traditional SRS approach of performing separate, independent simulations of parent nuclides should use caution when conducting simulations to establish disposal limits for particular facilities, especially if sufficient closure inventories for certain radionuclides are anticipated that might cause concentrations within the waste zone or other portions of the flow field to approach the corresponding water solubility limits. At the time of Rev. 1 of this report, improvements to the PORFLOW code have addressed this issue. The code now allows multiple isotopes to be simulated simultaneously. The problem described above is avoidable, providing the user is aware that multiple isotopes of the same element could approach the solubility limit and enables the solubility feature within PORFLOW.

2.7 Summary

The purpose of this exercise was to demonstrate whether or not the two codes implement the contaminant transport processes in a similar manner, before moving on to the second phase of benchmarking, which is discussed in Section 3.0. Considering the extremely close adherence of modeled results once identically configured flow domains, parameters and boundary conditions were incorporated within each code, it is judged that proceeding on to the 1D GoldSim benchmarking to 2D and 3D PORFLOW simulations is justified and that any differences in modeled results will not have originated in how each code implements the contaminant transport and radioactive decay processes.

3.0 PORFLOW 2D/3D Models to GoldSim 1D Model Benchmarking

Benchmarking was performed to show whether or not the GoldSim 1D model provided sufficiently similar results to the PORFLOW multi-dimensional models. If the results were sufficiently similar, one may infer that the response of the GoldSim model to the stochastic parameters reflects the physical system's response. This section describes the steps taken to perform the benchmarking.

Benchmarking is accomplished in three stages. First, the flow data are abstracted from PORFLOW. Second, the contaminant fluxes between the unsaturated and saturated zones are compared. This is considered a good spot to benchmark as the contaminant fluxes are what the PORFLOW 2D UZ model passes to the PORFLOW 3D SZ model. Third, contaminant concentrations are compared at the assessment point, in this case the 100m well. Contaminant concentrations are used as that is what is passed to the dose model by both transport models.

Benchmarking comparisons are made with the updated ST model, SRS ELLWF Slit Trench v1.2.gsm (Tauxe and Catlett, 2010) by comparing results obtained from that model against the PORFLOW ST model developed for the 2008 PA (WSRC, 2008).

3.1 PORFLOW Data Provided for Benchmarking

PORFLOW reference data (results) were obtained for two different unsaturated zone (UZ) simulation scenarios, Case01 and Case11 in the SRS PA. Case01 represents the condition where 100% of the emplaced waste is considered to be completely crushable. Case11 represents the condition whereby 100% of the waste is considered to be non-crushable. Non-crushable waste is assumed to withstand compaction, which occurs at the end of Institutional Control. Shortly after compaction and placement of the final closure cap over the ELLWF, the non-crushable waste is assumed to undergo complete corrosion and collapse, thus causing damage to the overlying closure cap and inducing a much higher rate of infiltration.

The SRS PA base case for the saturated zone is a blended scenario which assumes that the source term is derived from 90% of the waste being crushable (Case01) while 10% is non-crushable (Case11). This blended saturated zone base case was referred to as Case01n11.

While the PA PORFLOW simulation required that two UZ simulations be performed (Case01 and Case11), followed by a blending of the contaminant fluxes to provide the appropriate source terms for use with the 3D SZ model, GoldSim has parallel UZ flow columns so that the blended source term can be modeled in a single simulation. Thus, flow fields were calculated in PORFLOW for both the 100% crushed and the 100% non-crushed cases and provide the flow information needed to establish the appropriate flow term in each of the parallel UZ columns in GoldSim.

The timeline of events is the same (i.e., Operational and Institutional Control periods are identical) for the crushable (Case01), non-crushable (Case11) and blended (Case01n11) cases up to the time of compaction and final closure (130 years). As a result, radionuclide release and transport will look the same for all three cases up until compaction and final closure takes place. This behavior will be shown by the contaminant flux and concentration history curves provided later in this report.

3.1.1 *Flow Data Abstraction*

GoldSim does not provide a flowfield calculation, therefore the flowfield from the multi-dimensional PORFLOW model must be abstracted to the 1D model. PORFLOW uses a 2D model in the unsaturated zone and a 3D model in the saturated zone. The following sections described the abstraction of flow data from those two different PORFLOW models. The PORFLOW 2D flow model is run as 36 steady-state flow calculations, with each calculation representing a period in time. The flow in the saturated zone is assumed to be constant in time.

3.1.2 *Unsaturated Zone Flow Abstraction*

Figure 3-1 shows the computational grid used in the PORFLOW simulations of the unsaturated zone. The circled nodes are where flow data were extracted. The GoldSim model is conceived to be 1D in the vertical direction, or, in the node-parlance of PORFLOW, the j-direction. The paradigm for the abstraction is that each horizontal level, which consists of five points, will have the same flow. In addition, previous benchmarking exercises have shown that a geometric average of the vertical stack provided a sufficiently good result (for Slit Trenches). Although PORFLOW shows the flow to be fairly consistent in the vertical direction for slit trenches, a vertical stack of nodes is needed for the transport calculation for issues such as numerical dispersion. Figure 3-2 shows the results of the abstraction. The “j=” corresponds to the levels (rows). Each j-value is a geometric average of the five values at that level. The solid line in Figure 3-2 is the geometric average that was used in the benchmarking.

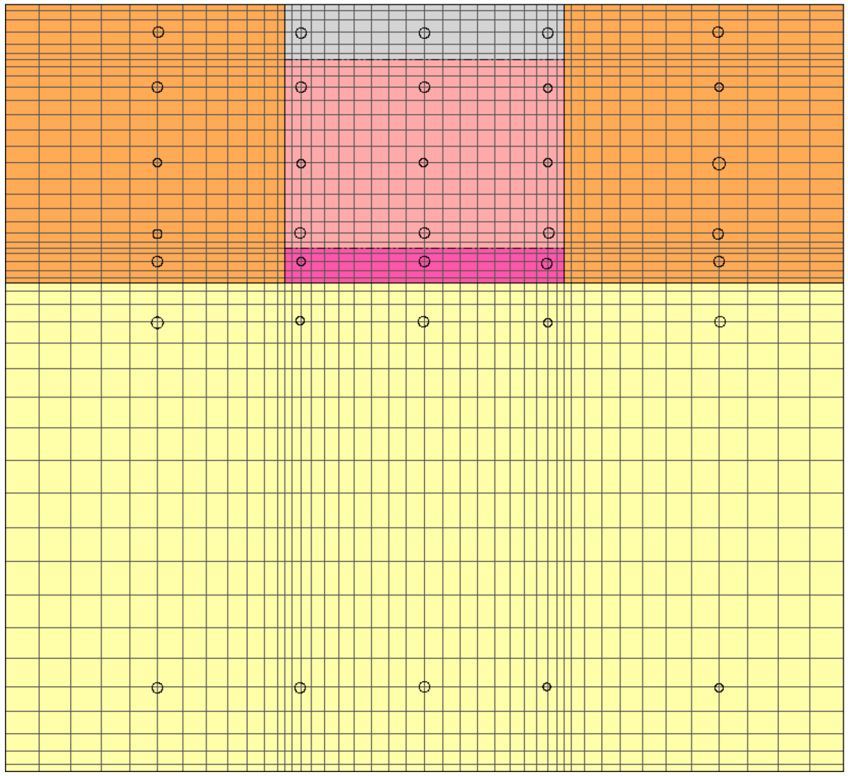

Figure 3-1. Flow Abstraction Points

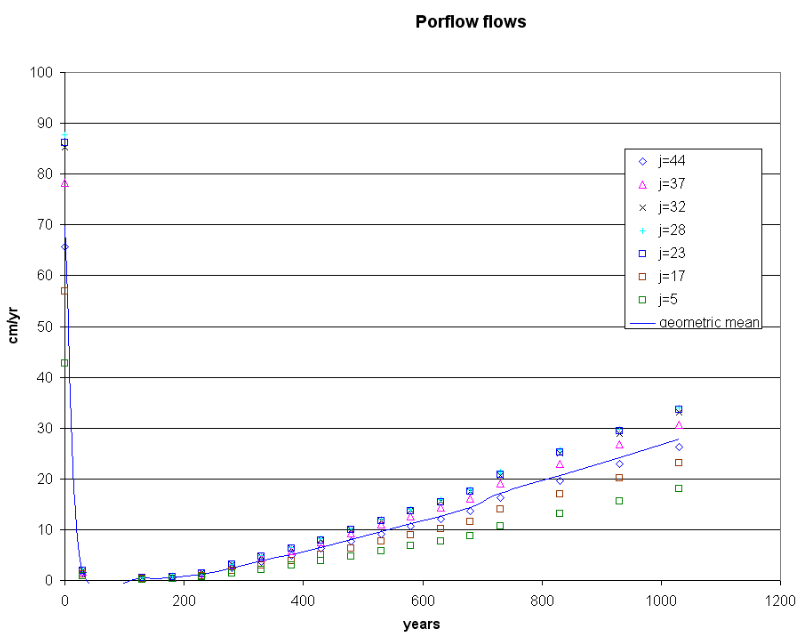

Figure 3-2. Abstracted Flow Data

3.1.3 *Saturated Zone Flow Abstraction*

The saturated zone (SZ) flow abstraction is approached differently from the unsaturated zone. The important event in the saturated zone is the timing of the arrival of the contaminant at the assessment point. The timing is controlled by the velocity of the flowfield. In GoldSim, a conservative tracer is run through the model and the velocity used in the saturated zoned is adjusted to correspond to the arrival time of the peak concentration of a conservative tracer in PORFLOW. Note that at this time the value of the concentration is not of interest, only its arrival time.

3.2 Unsaturated-Saturated Contaminant Flux Benchmarking

Benchmarking at the UZ-SZ contaminant flux boundary was accomplished by comparing the flux profiles of five parent radionuclides and their progeny. The parents selected, based on their contribution to dose, were ^{99}Tc, ^{3}H, ^{14}C, ^{237}Np, and ^{239}Pu. The first four have relatively low K_d values while the last does not. Low distribution coefficient values typically lead to easy benchmarking, while high values can point to issues with the modeling. The significance of this will be discussed in the following sections.

In some ways the PORFLOW analysis is a pseudo-1D model. A single value of contaminant flux is supplied to the saturated zone model from the unsaturated zone model. The flux which is passed between models is the total flux, that is, the flux leaving all faces of the 2D computational grid. This greatly simplifies the benchmarking in that one need only be concerned with the total flux, so if one can match that, one is passing an equivalent amount of contaminant.

3.2.1 *GoldSim Benchmarking Adjustments*

To achieve relatively close conformance of results between fluxes generated by the two codes, two GoldSim model input variable adjustments were needed for benchmarking purposes. The simplest one was applying a factor of 0.8 to all the velocities. The following applies to both cases and to the unsaturated zone (as it is discussing fluxes). This was determined by examining the flux curves for the two non-retarded species, ^{14}C and ^{3}H. With this accomplished, the fluxes for the retarded species, especially ^{239}Pu, which has the highest distribution coefficient, were still not in good agreement with respect to peak fluxes. One observation was that the GoldSim fluxes show more compact peaks, with higher magnitudes and narrower spreads. When looking at differences in the two models, it became readily apparent that there was a noding difference between the two. In the zone between the waste and the saturated zone, the GoldSim model had 30 nodes while the PORFLOW model had 20 nodes to represent that region of its domain. When the GoldSim model was changed to match the PORFLOW model by reducing the number of nodes to 20, the discrepancies disappeared. This noding exercise demonstrated that noding is an important issue for both models.

3.2.2 *Time Steps*

As the benchmarking began, the apparently anomalous behavior of ^{237}Np (Figure 3-3) was obvious. Initially, it appeared there was a difference in the total mass exiting the UZ, so an integration of contaminant mass in GoldSim data was performed. The integrated masses of ^{237}Np leaving the UZ in the GoldSim and PORFLOW simulations are shown in the left frame Figure 3-4. The total masses for GoldSim and PORFLOW are, respectively, 258.32 g and 237.18 g. The GoldSim results did not seem plausible considering that the initial mass was 237 g. These initial GoldSim results were generated with the time steps supplied by Neptune and Company, which were then reduced in length to 0.5 years for the first 500 years to generate the graph on the right-hand frame of Figure 3-4. Using the shorter time-steps the final GoldSim integrated mass for ^{237}Np is 236.98 g. Having established that the modified time-steps produced more accurate results, they were retained for the remainder of the analyses. Reference PORFLOW output was generated using a 0.1-yr time-step for ^{14}C, ^{3}H and ^{99}Tc simulations and a 1-yr time-step for ^{237}Np and ^{239}Pu simulations. These time-steps were kept constant throughout the simulations. Although the GoldSim and PORFLOW time-stepping schemes used for this comparison were not identical, they were sufficiently similar to produce highly similar mass fluxes from both models. It is expected that if identical time-steps had been employed, then nearly identical mass fluxes would have resulted. If further time-stepping evaluation is conducted, this assertion should be verified.

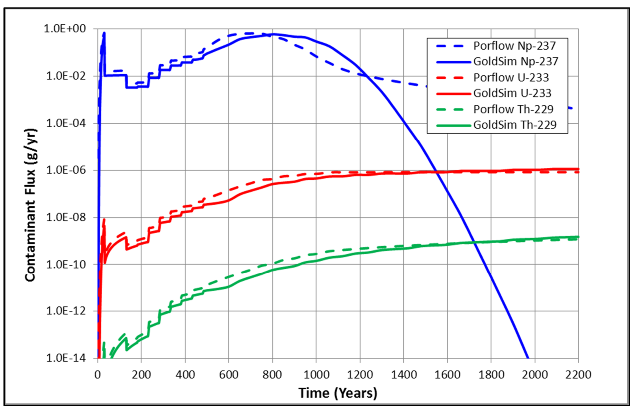

Figure 3-3. Case11 ^{237}Np Behavior

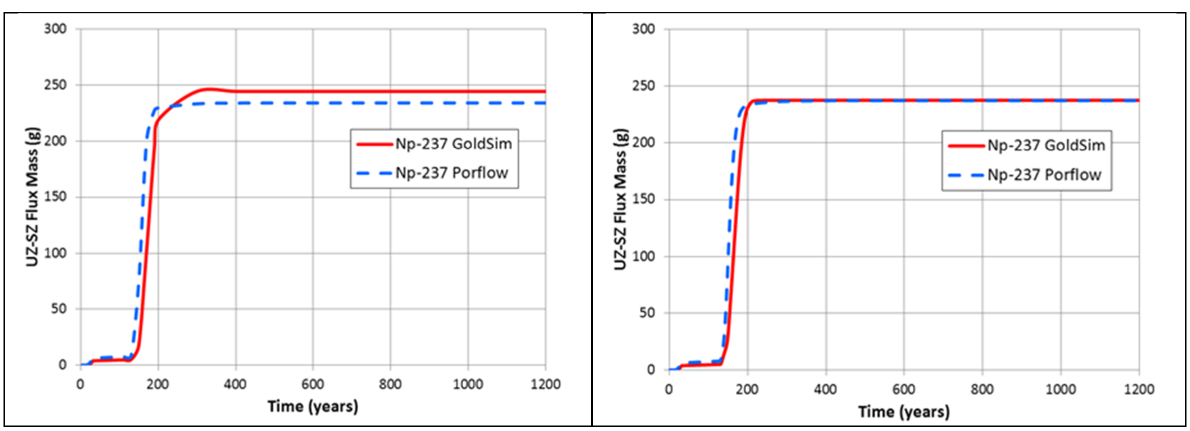

Figure 3-4. Time Step Effect

3.2.3 *Case11*

Case11 allows for a straightforward comparison because it is self-contained. There is no blending of fluxes, the PORFLOW simulation is run as though 100% of the waste is non-crushable.

The UZ-SZ flux comparisons for Case11 are illustrated in Figures 3-5 to 3-9. The fast-moving radionuclides, ^{3}H, ^{99}Tc, and ^{14}C show quite good agreement. A drop-off in the concentration of ^{237}Np after 220 years is caused by a difference in the integrated mass of 2 g, or less than 1%. Basically, the GoldSim simulation runs out of mass before the PORFLOW simulation. As shown above, PORFLOW has mass in excess of the initial mass due to its time-stepped induced mass error. At 220 years, where the crossover of the GoldSim and PORFLOW curves occurs, the integrated masses of ^{237}Np are 236.8 g and 234.7 g, respectively. The ^{239}Pu family shows fairly good agreement with matching trends. The total mass ^{239}Pu having left the system at 2200 years is 0.016 g.

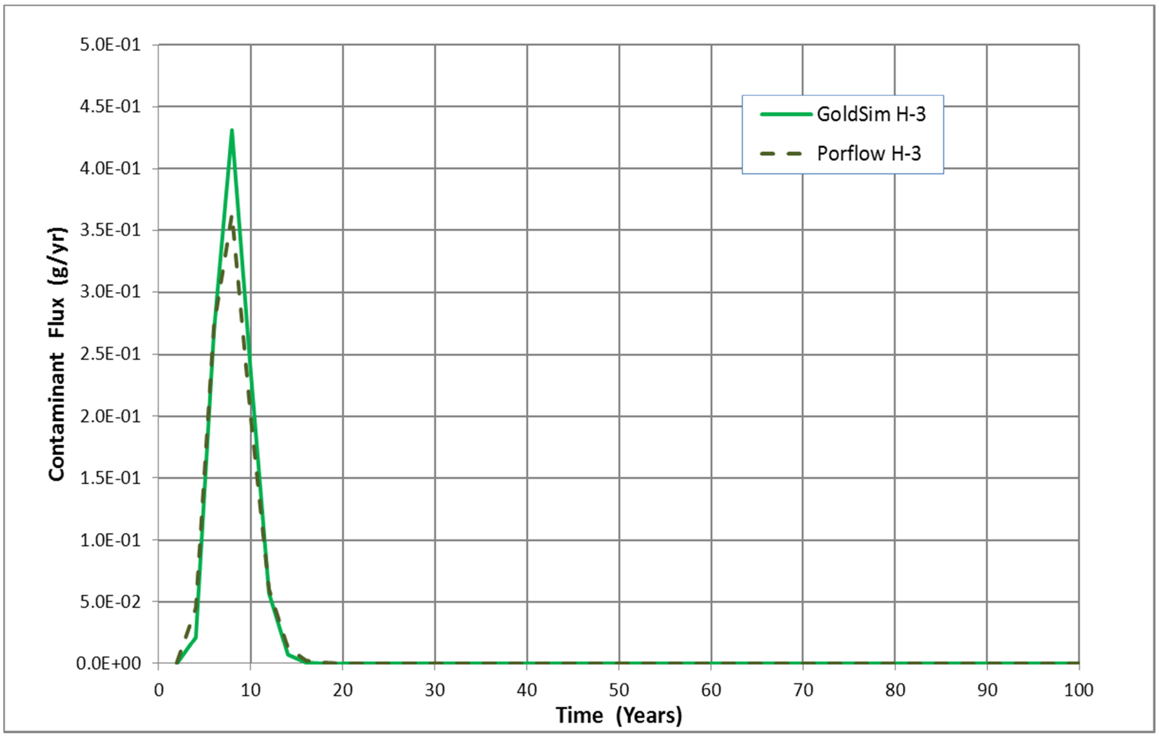

Figure 3-5. Case11 UZ-SZ Flux Comparisons for ^{3}H

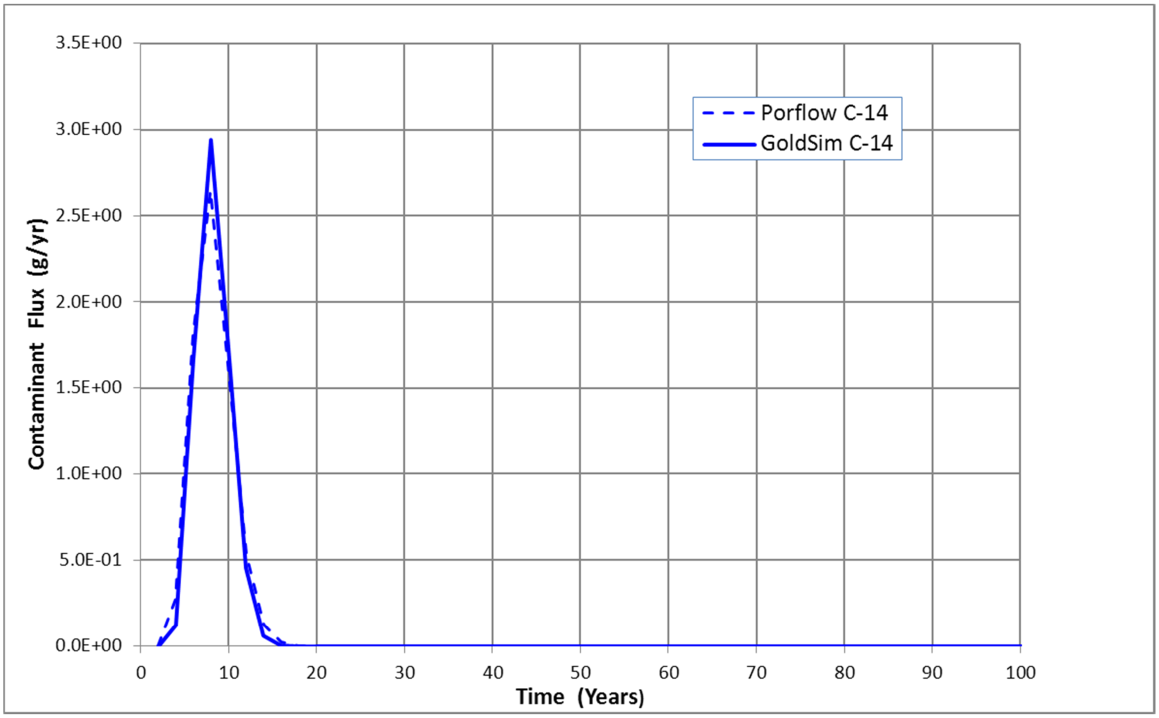

Figure 3-6. Case11 UZ-SZ Flux Comparisons for ^{14}C

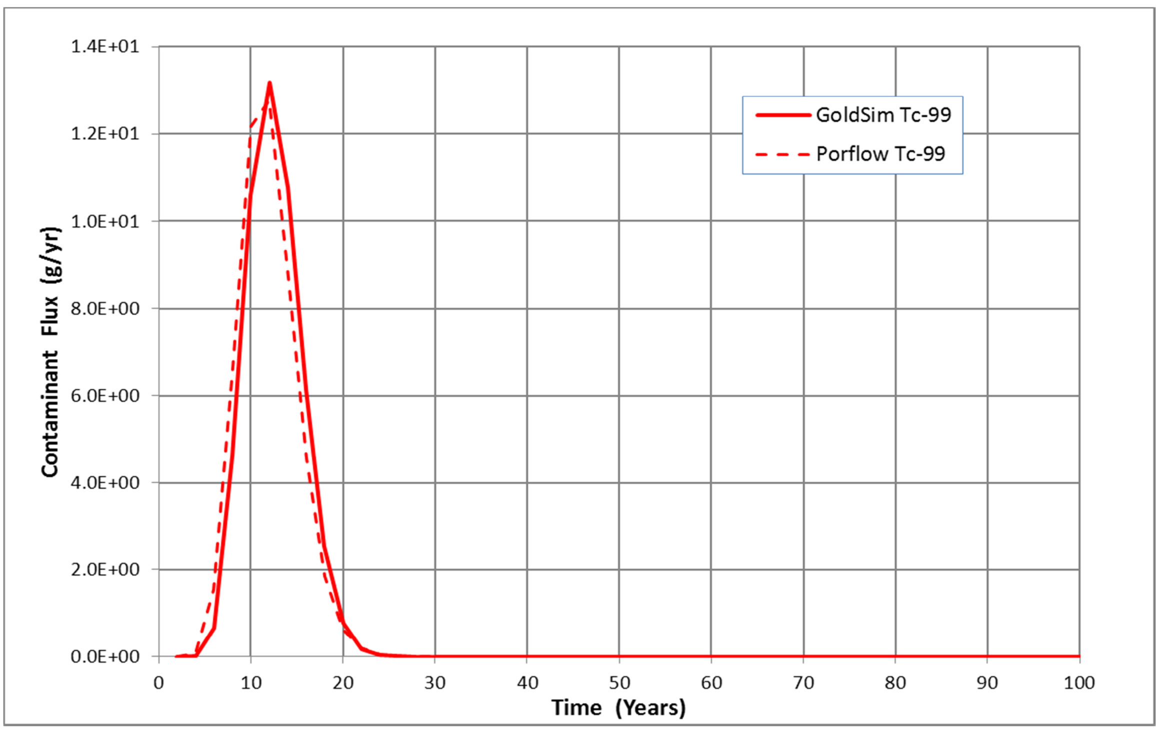

Figure 3-7. Case11 UZ-SZ Flux Comparisons for ^{99}Tc

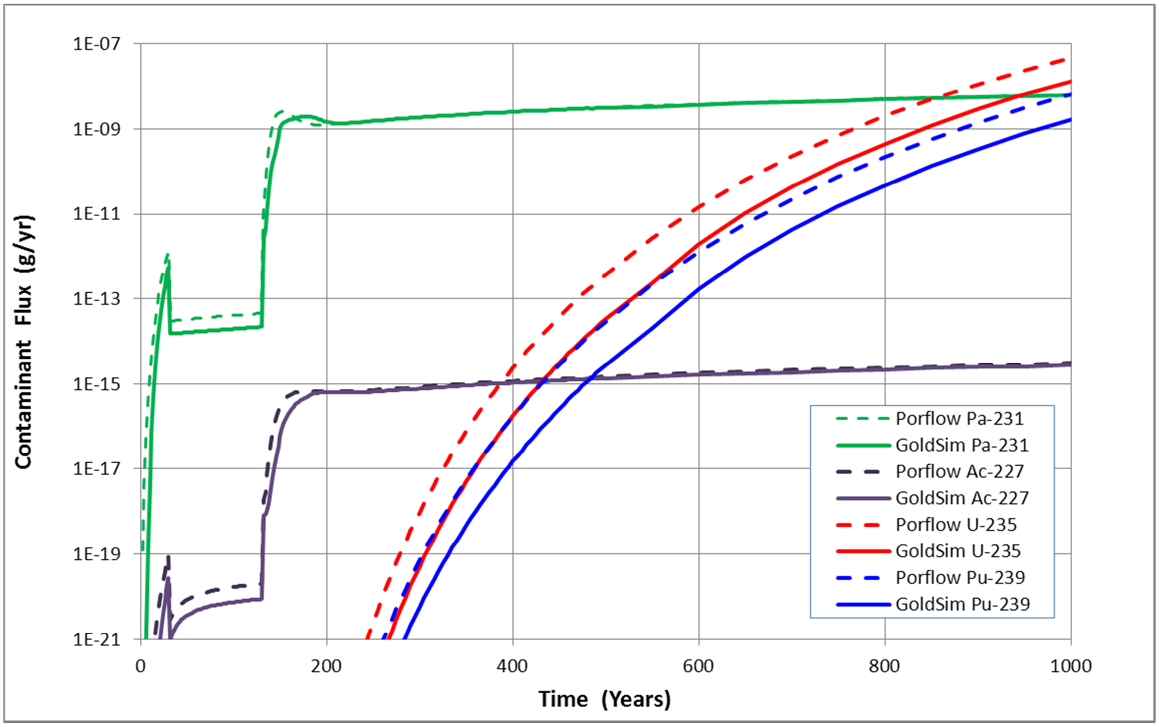

Figure 3-8. Case11 UZ-SZ Flux Comparisons for the ^{239}Pu Family

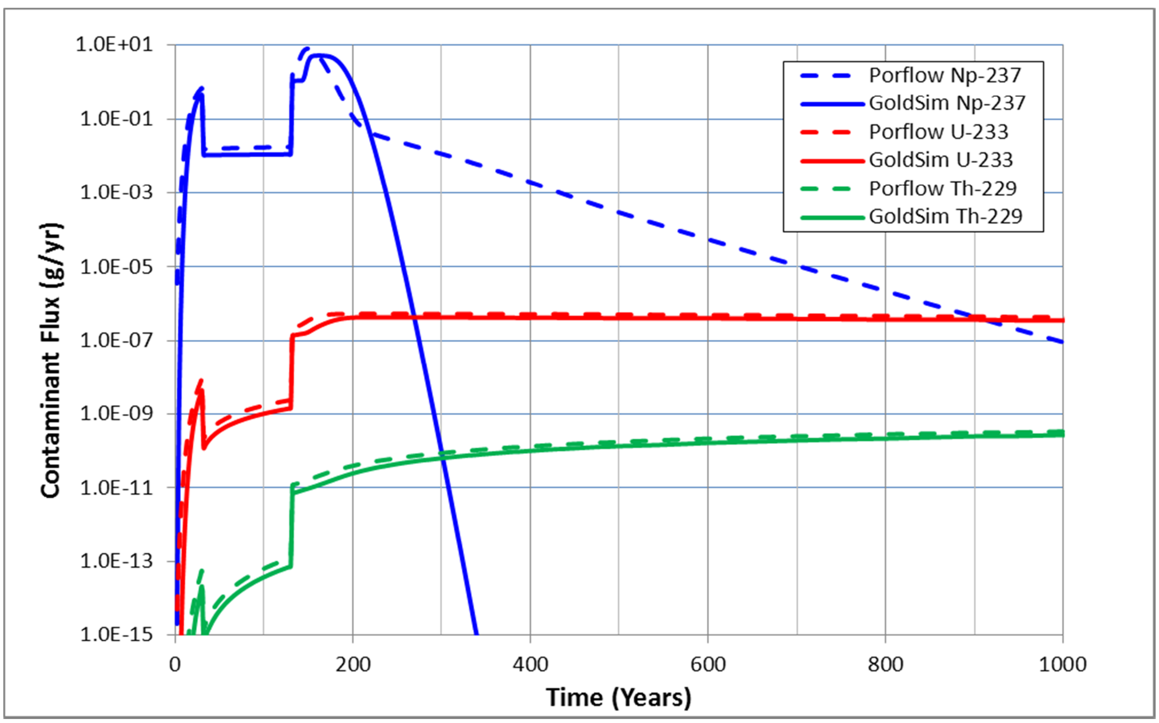

Figure 3-9. Case11 UZ-SZ Flux Comparisons for the ^{237}Np Family

3.2.4 *Case01*

The infiltration data supplied for this benchmarking exercise assumed 100% crushed waste. The following comparisons will be comparing 100% crushed waste from both the PORFLOW and GoldSim simulations. The UZ-SZ flux comparisons for Case01 are illustrated in Figures 3-10 to 3-14. No additional adjustments to the Section 3.2.1 input parameter adjustments were applied to the model. Good agreement is seen for all the radionuclides with the exception of ^{237}Np after 1200 years. See the discussion of ^{237}Np behavior in Section 3.2.3 for an explanation.

The timeline of events is the same (i.e., Operational and Institutional Control periods are identical) for the crushable (Case01) and non-crushable (Case11) cases up to the time of compaction and final closure (i.e., 130 years). As a result, the Case01 and Case11 contaminant flux curves are the same for ^{3}H, ^{14}C and ^{99}Tc because they peak prior to compaction and final closure. However, differences can be seen between Case01 and Case11 fluxes for the family of ^{239}Pu and ^{237}Np curves as these parent nuclides and their progeny peak after final closure.

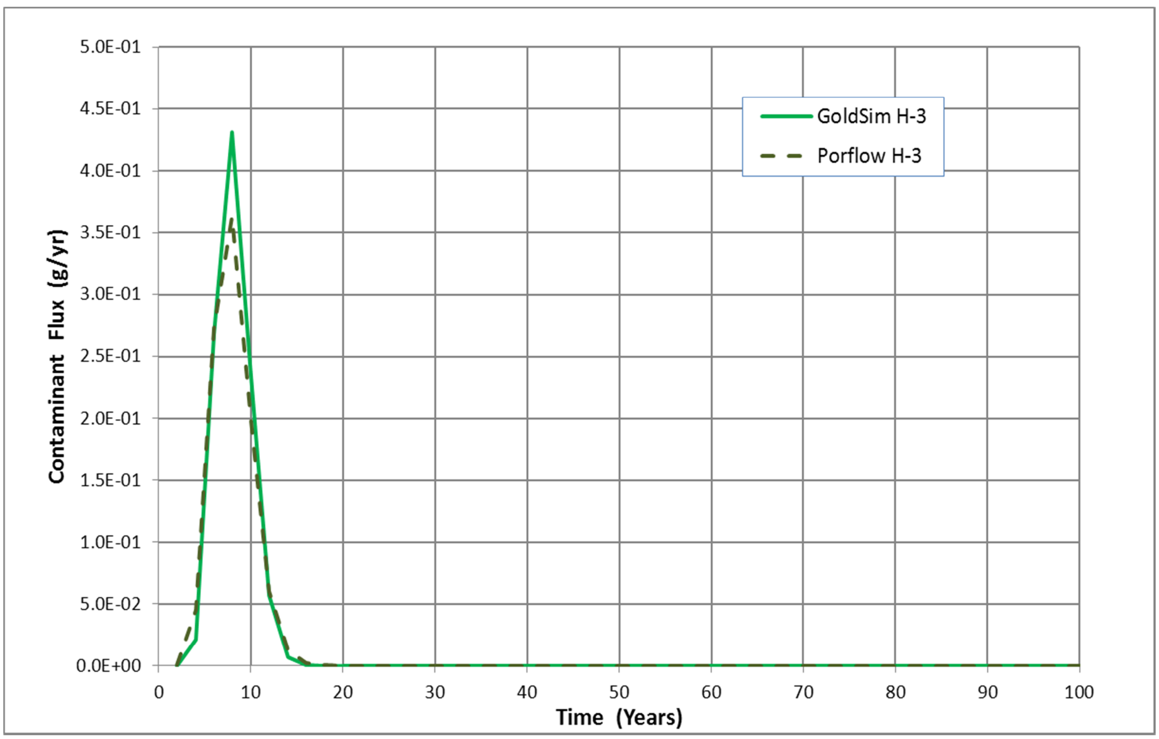

Figure 3-10. Case01 UZ-SZ Flux Comparison for ^{3}H

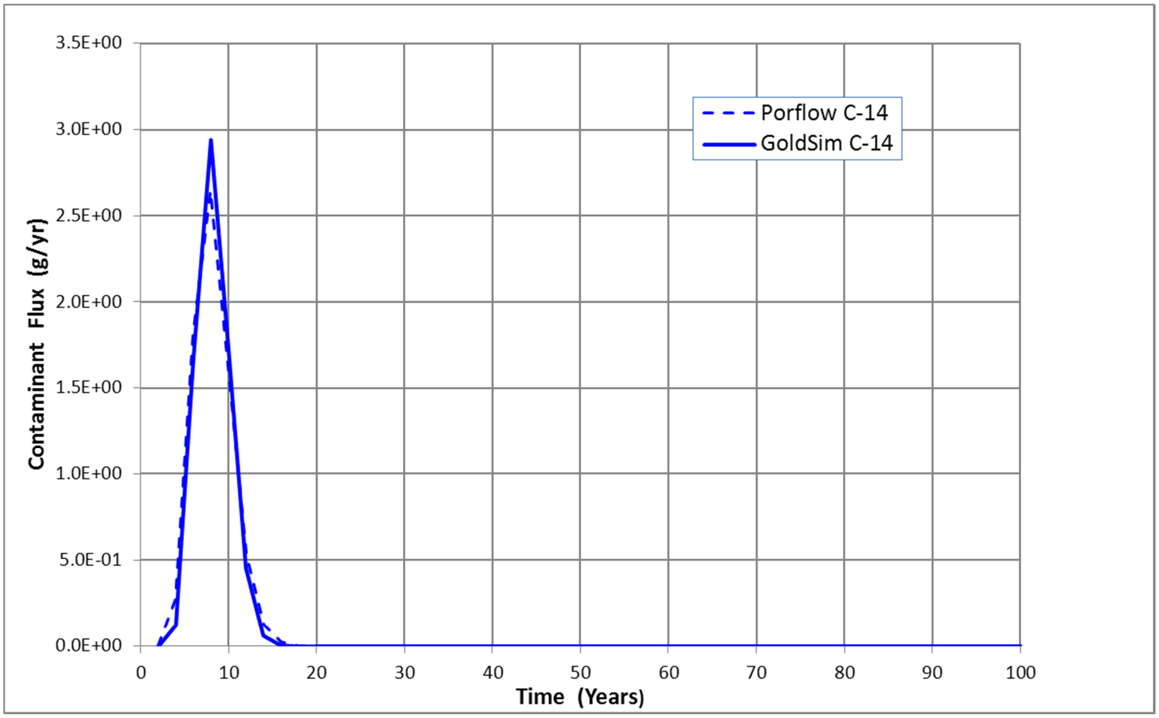

Figure 3-11. Case01 UZ-SZ Flux Comparison for ^{14}C

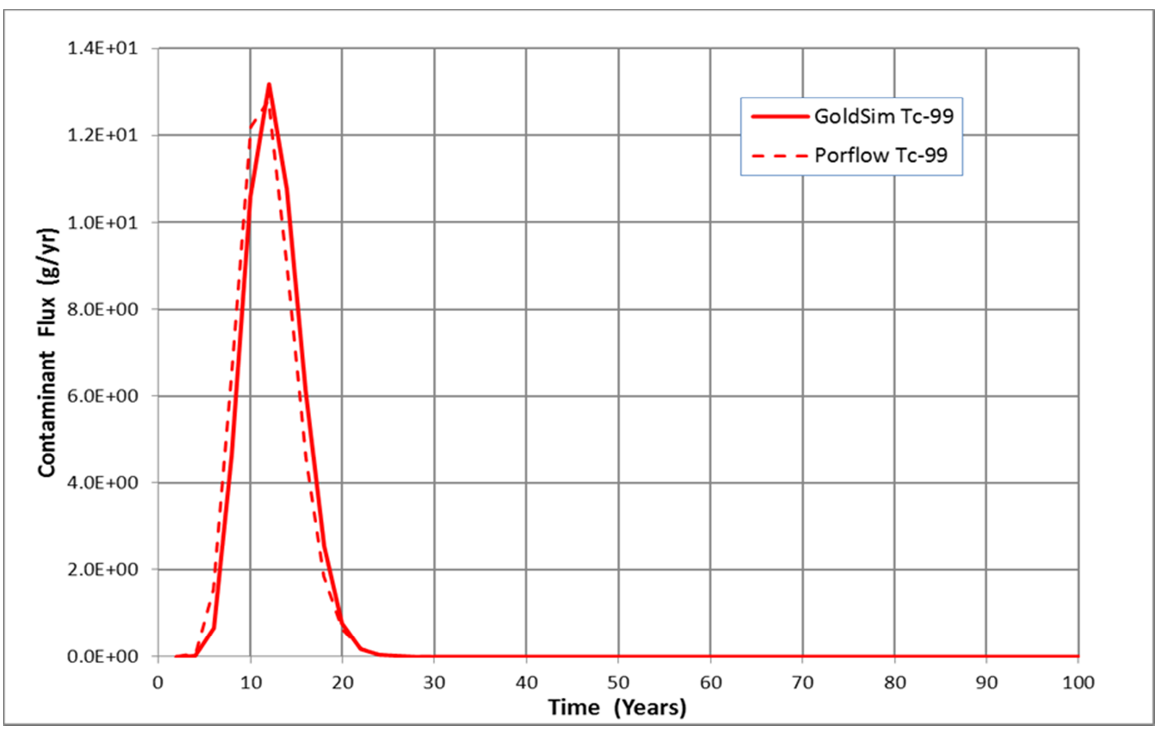

Figure 3-12. Case01 UZ-SZ Flux Comparisons ^{99}Tc

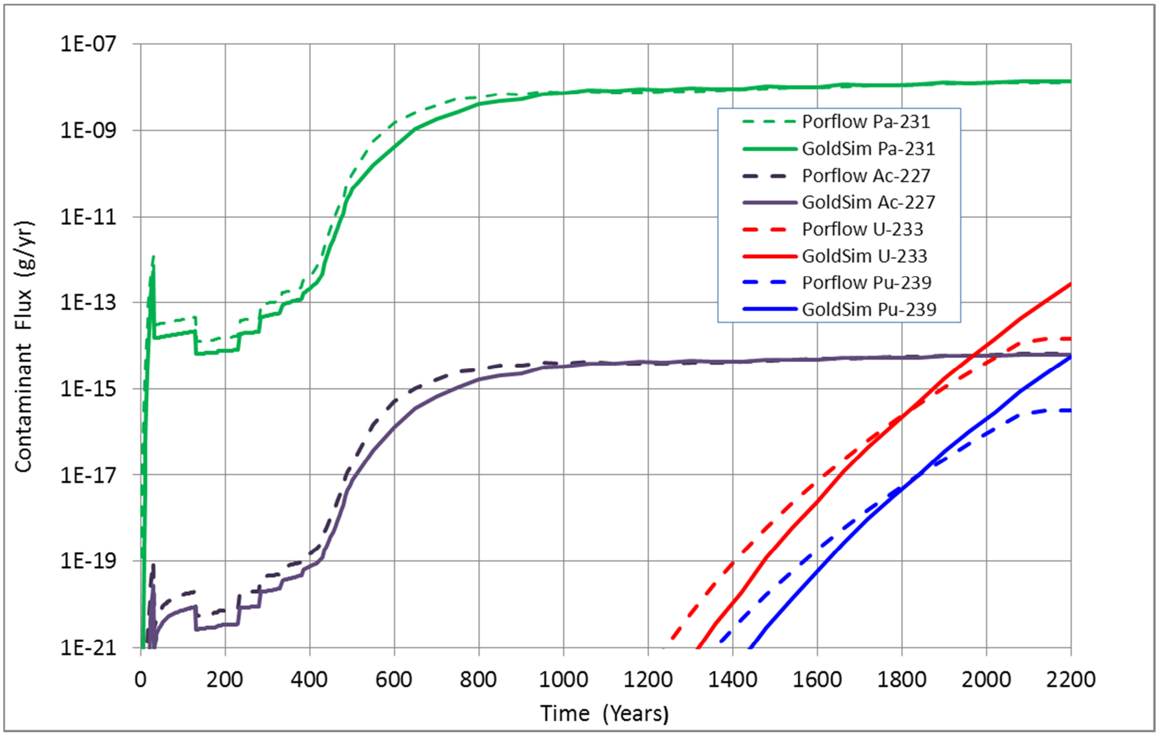

Figure 3-13. Case01 UZ-SZ Flux Comparisons for the ^{239}Pu Family

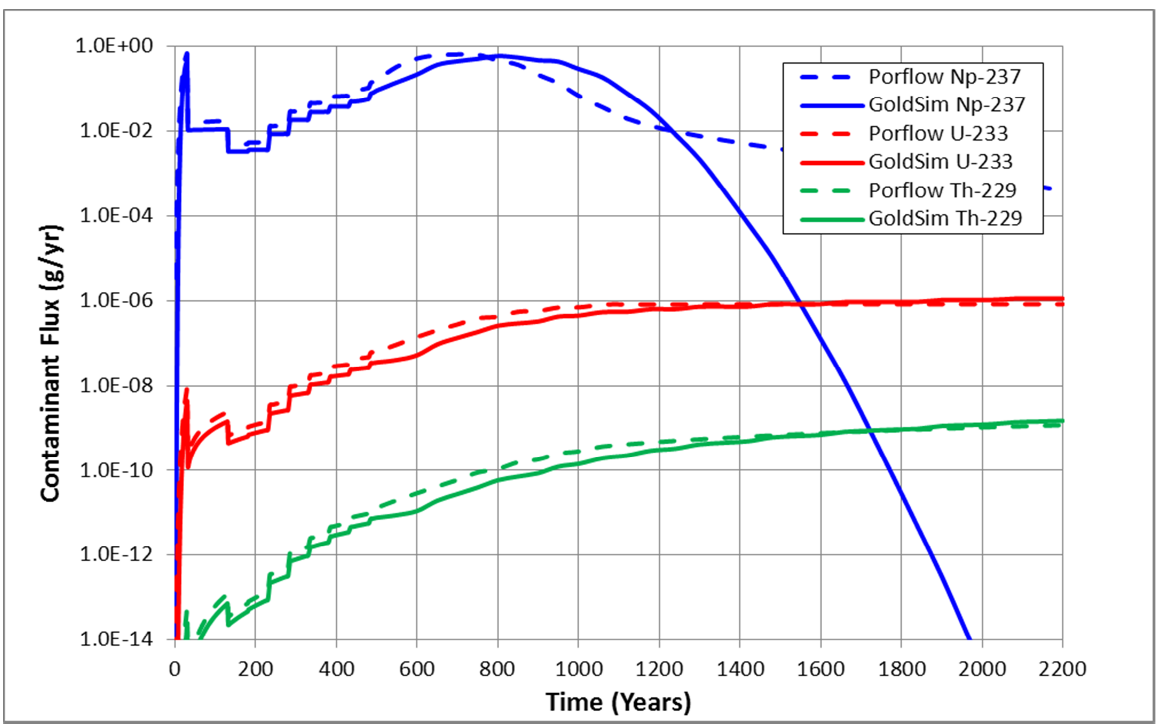

Figure 3-14. Case01 UZ-SZ Flux Comparisons for the ^{237}Np Family

3.3 Compliance Point Benchmarking

The compliance point benchmarking was accomplished by comparing the GoldSim-generated concentration with the PORFLOW values. PORFLOW uses a compliance "zone." It samples all computational cells in a defined set of computational cells (a defined zone) to determine a groundwater plume maximum and plume average concentration. Two Cases were evaluated: Case01 which is the case where all waste was considered crushable; and Case01n11, where the source term was blended from 90% crushable waste and 10% non-crushable waste.

3.3.1 *GoldSim Benchmarking Adjustments*

No GoldSim input parameter adjustments were required in the saturated zone model to obtain adequate conformance of its output with PORFLOW results. The Darcy velocity was set to a representative value of 175 ft/yr and the saturated zone thickness was set to a representative value of 60 ft for both models.

3.3.2 *Case01n11*

The Case01n11compliance point groundwater concentrations computed in GoldSim are plotted against the PORFLOW calculated maxima and averages in Figures 3-15 to 3-19. GoldSim uses a single cell to compute a cell-centered average value of the concentration. Thus, having the GoldSim calculation lie between the PORFLOW maximum and average values demonstrates that the GoldSim model provides an adequate representation of the PORFLOW results. The only notable deviation is in the behavior of ^{237}Np, which is not unexpected because of its behavior in the UZ. It should be recalled that the difference in behavior is caused by less than a 1% difference in the integrated mass flux. One should note that for ^{237}Np and ^{239}Pu, the y-axis is truncated at about 1 atom/liter of the parent.

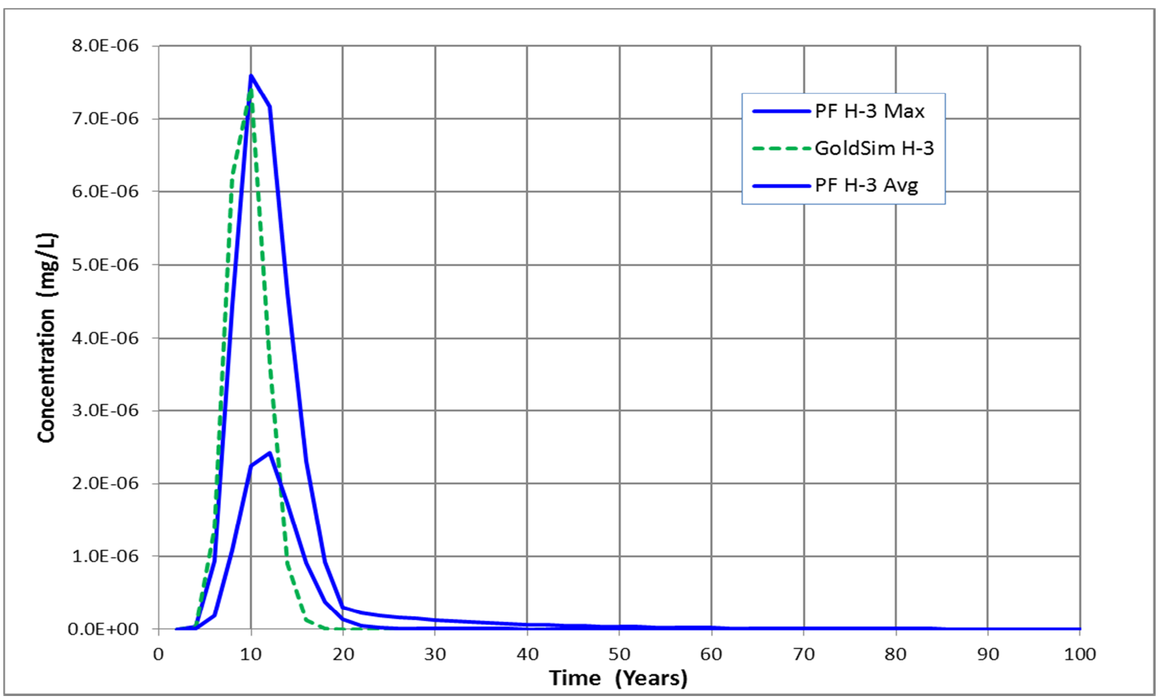

Figure 3-15. Case01n11 Compliance Point Comparisons for ^{3}H

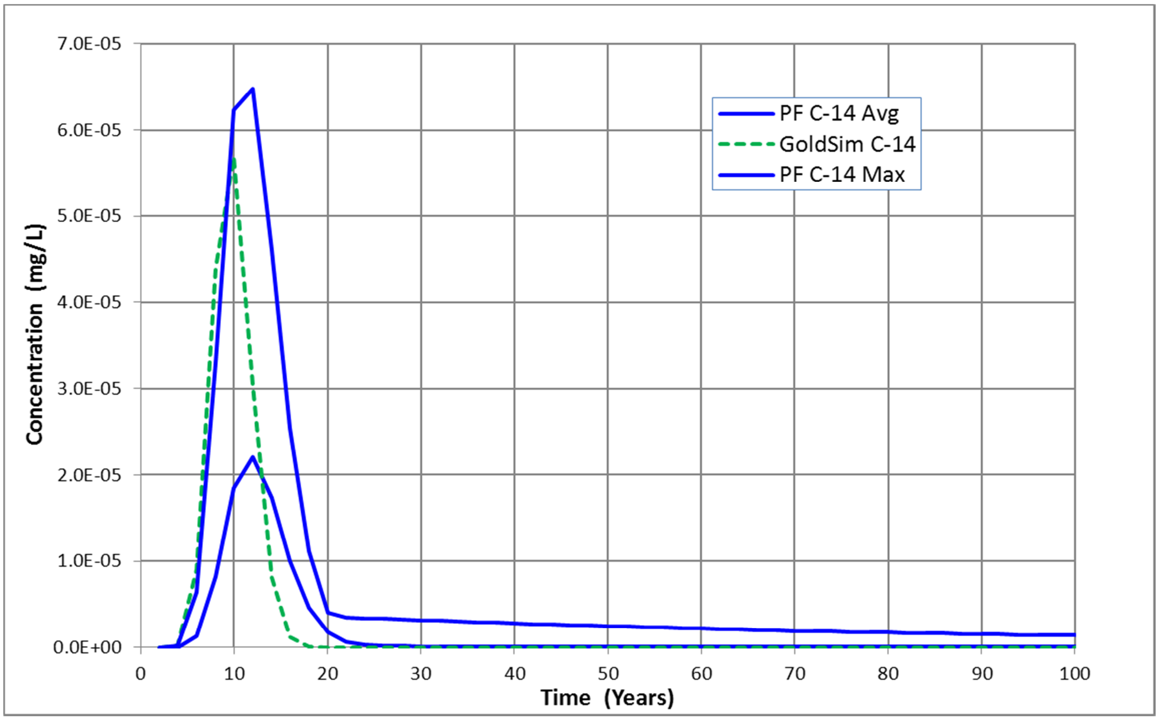

Figure 3-16. Case01n11 Compliance Point Comparisons for ^{14}C

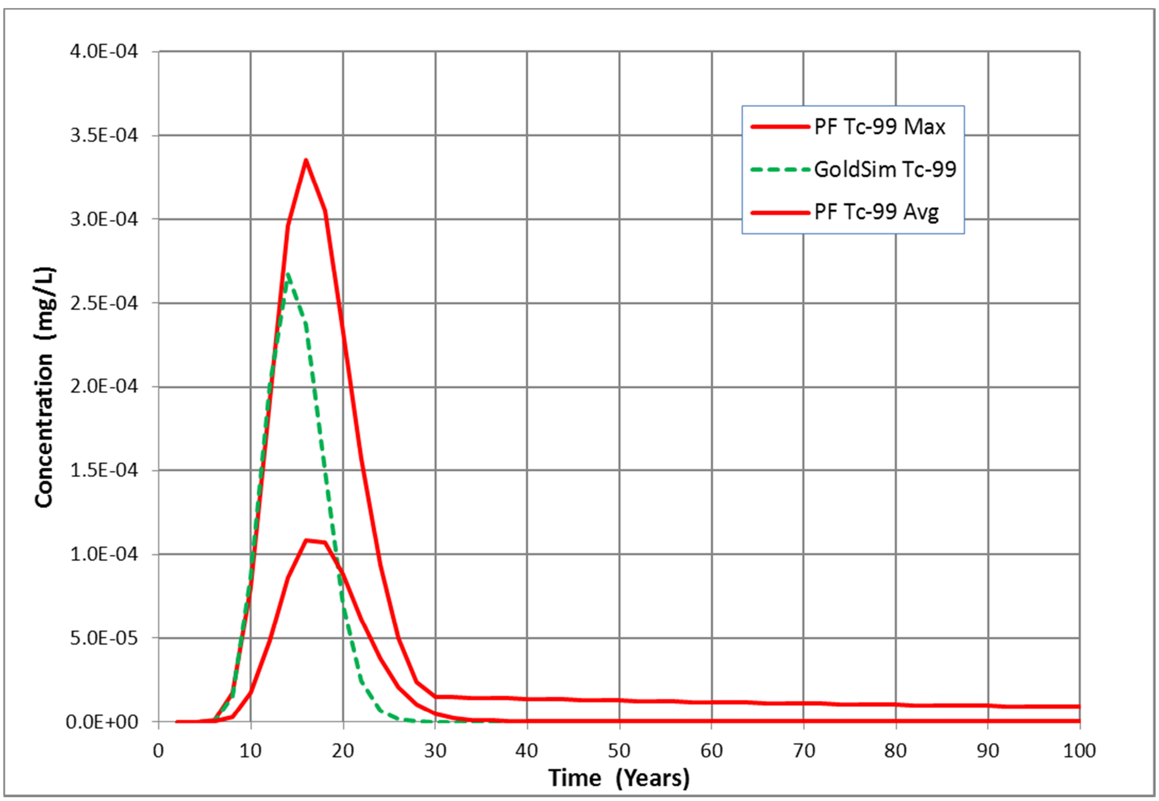

Figure 3-17. Case01n11 Compliance Point Comparisons for ^{99}Tc

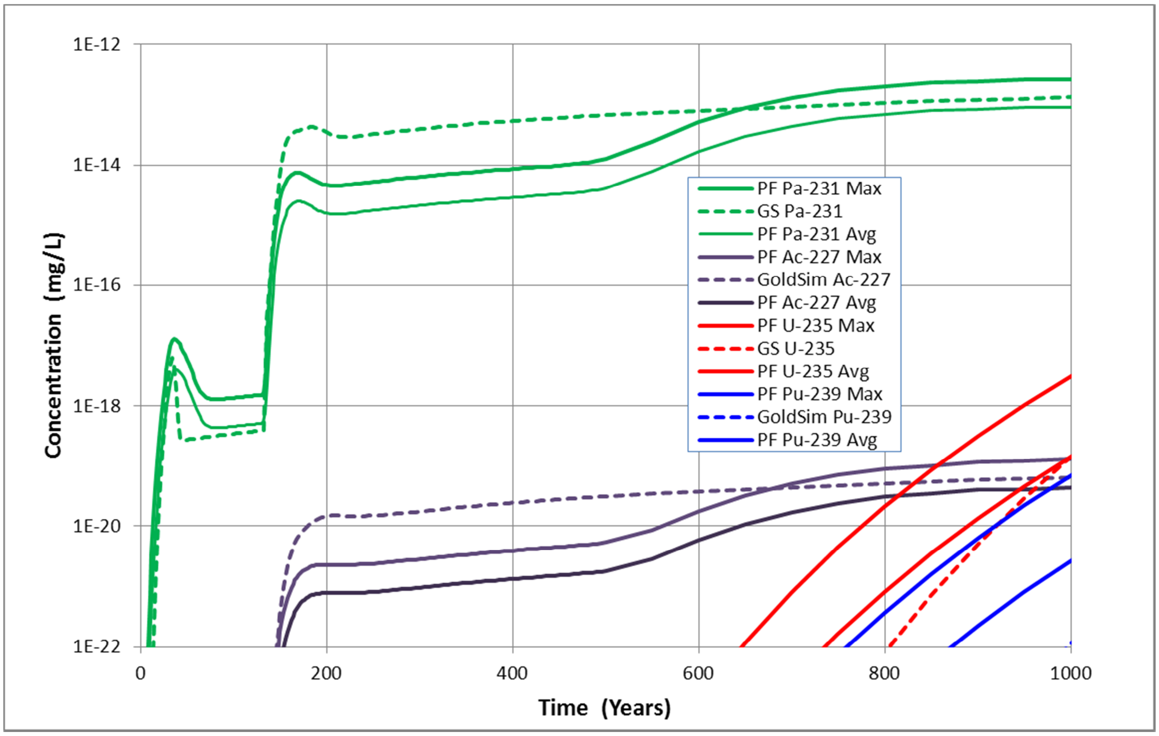

Figure 3-18. Case01n11 Compliance Point Comparisons for the ^{239}Pu Family

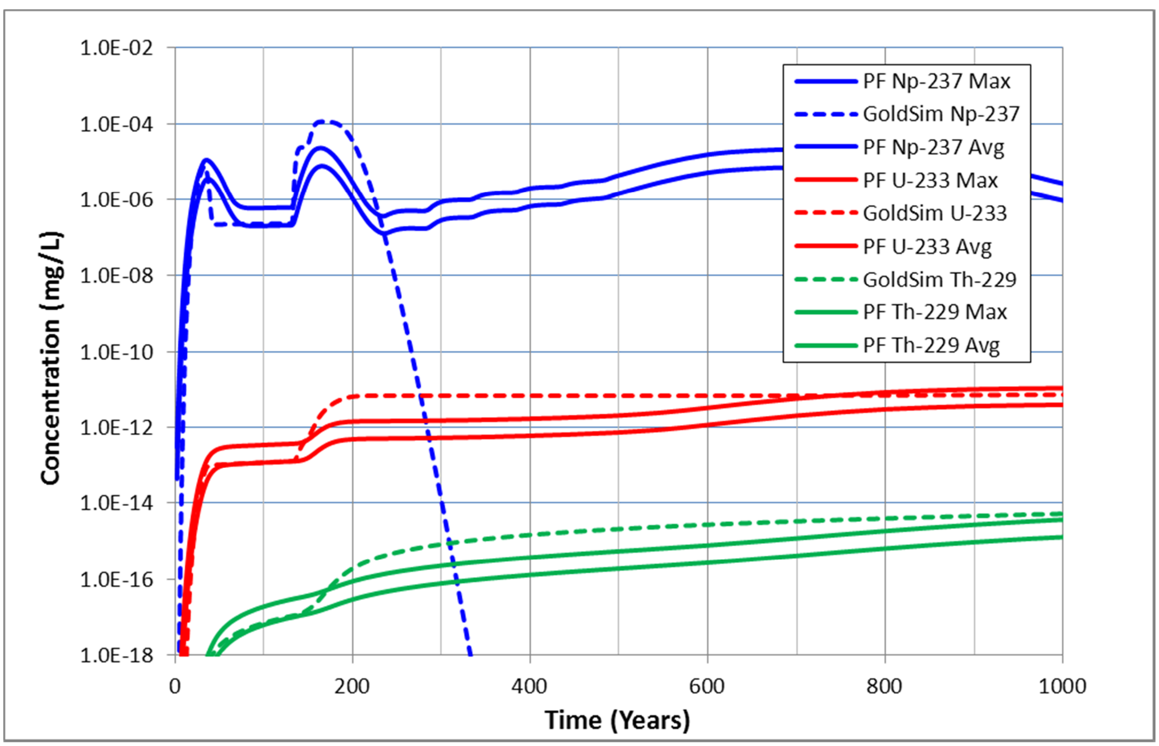

Figure 3-19. Case01n11 Compliance Point Comparisons for the ^{237}Np Family

3.3.3 *Case01*

The Case01compliance point groundwater concentrations computed in GoldSim are plotted against the PORFLOW calculated maxima and averages in Figures 3-20 to 3-24. This case provides mixed results. No ^{239}Pu appears at greater than 1 atom/liter. ^{99}Tc and ^{237}Np results fall between the maximum and average PORFLOW computed values. ^{3}H is transported more quickly by GoldSim, but when the curves diverge, it is on the order of 10^{-10} g/L, a rather insignificant amount. The same is true for ^{14}C. Its curves begin to diverge at about 10^{-9} g/L.

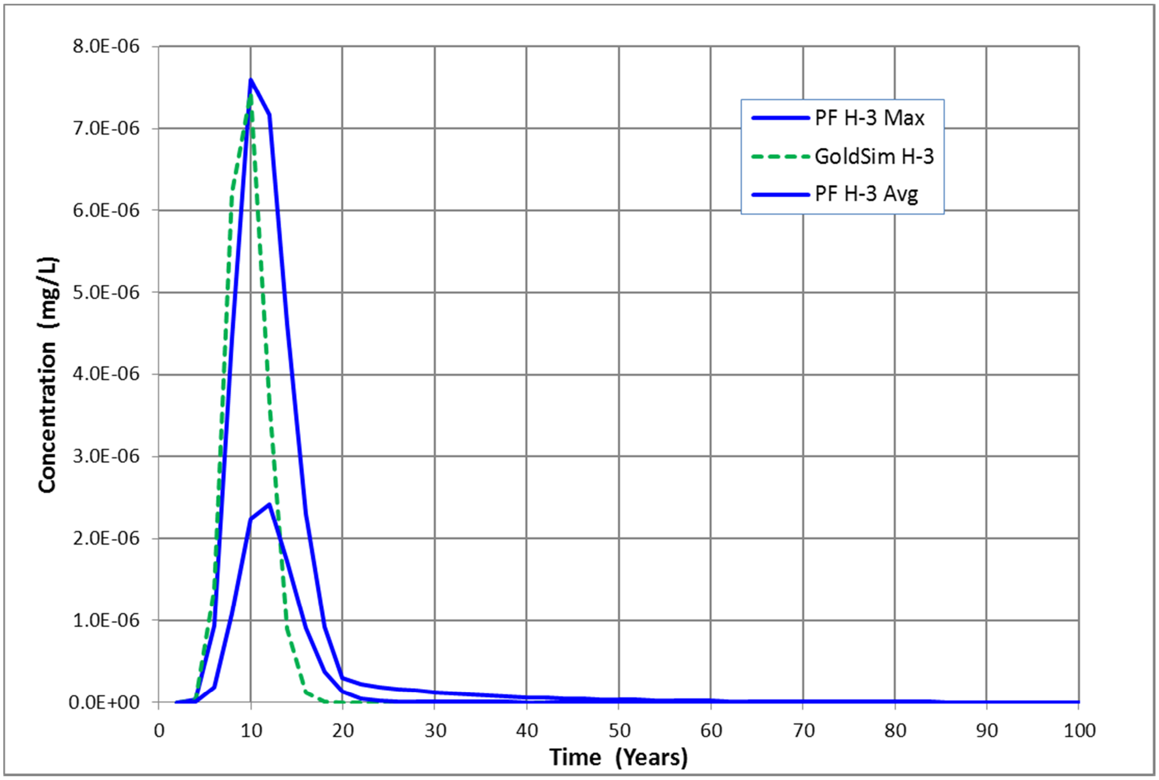

Figure 3-20. Case01 Compliance Point Comparisons for ^{3}H

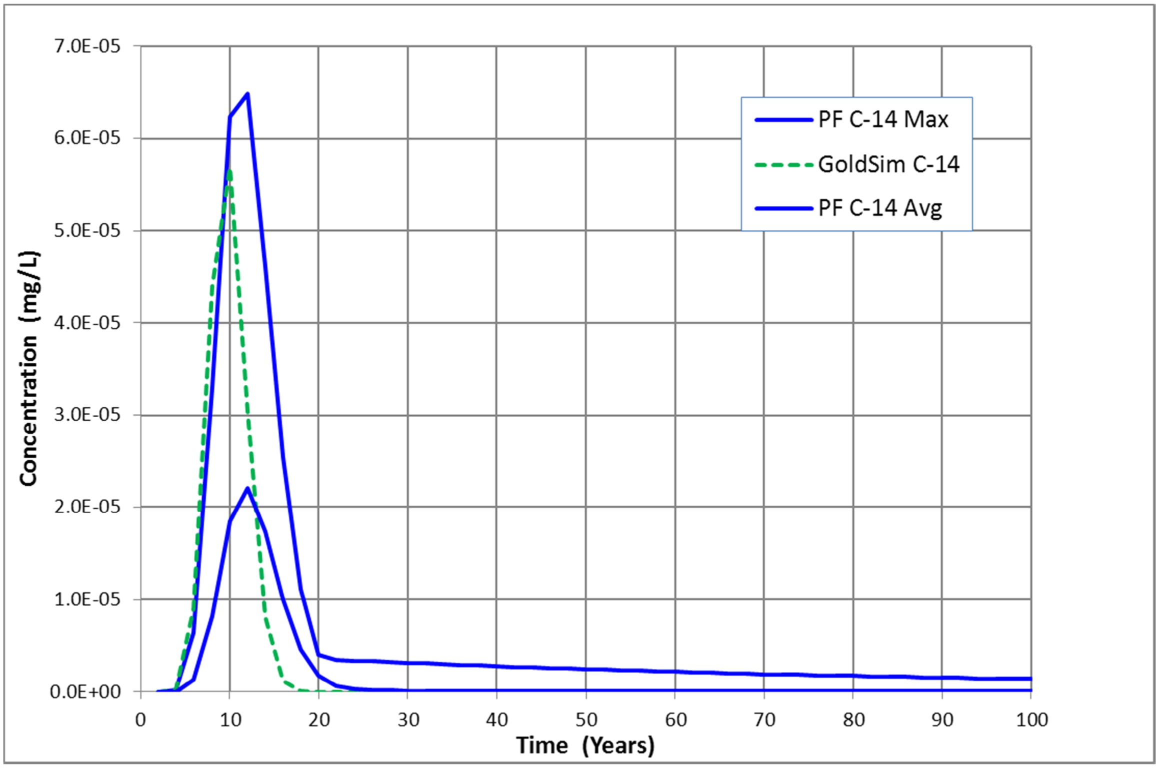

Figure 3-21. Case01 Compliance Point Comparisons for ^{14}C

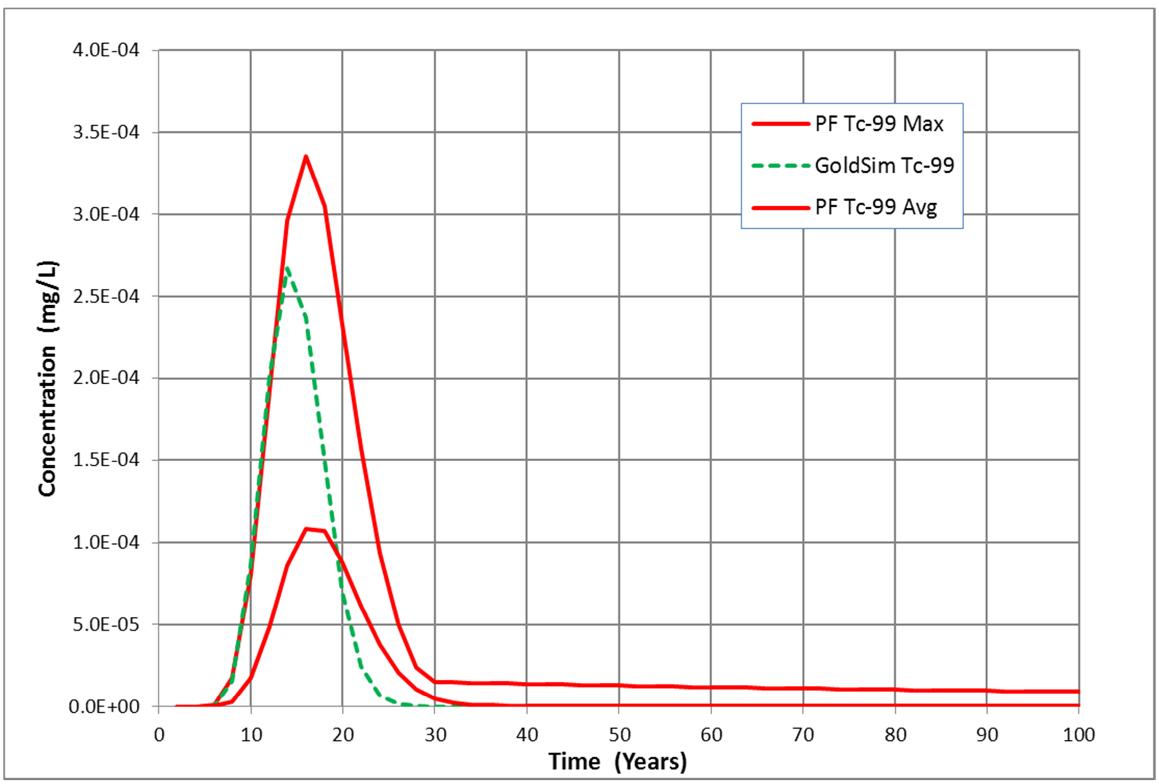

Figure 3-22. Case01 Compliance Point Comparisons for ^{99}Tc

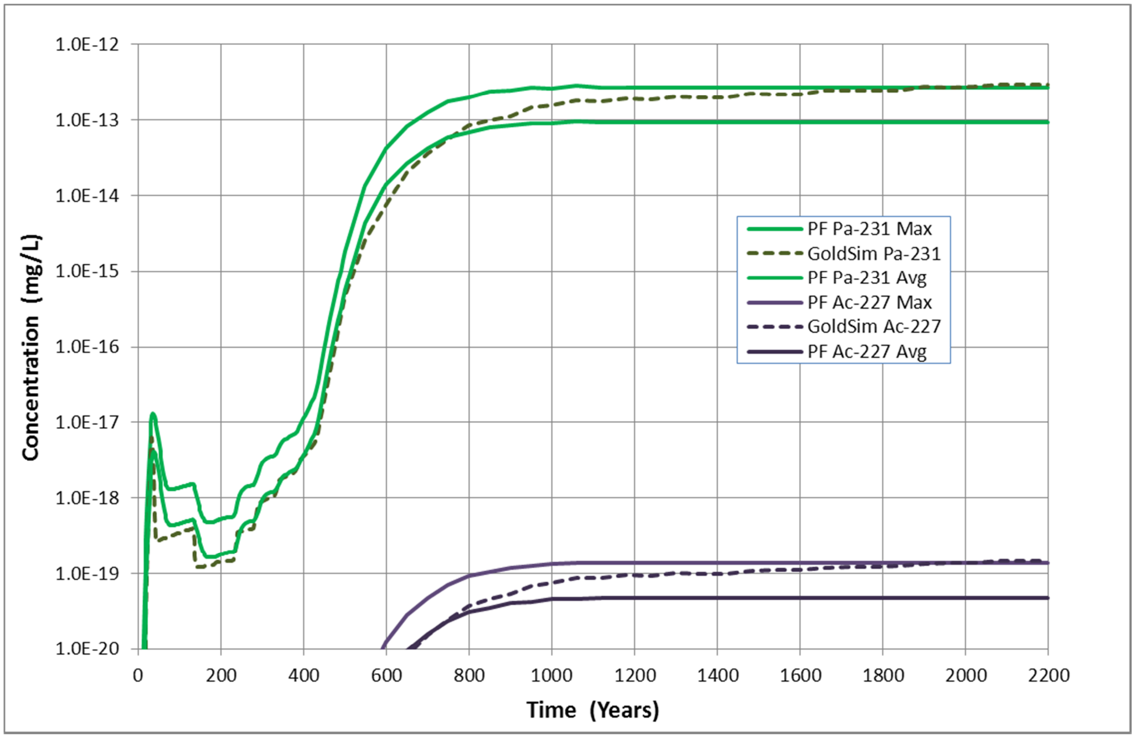

Figure 3-23. Case01 Compliance Point Comparisons for ^{239}Pu Family

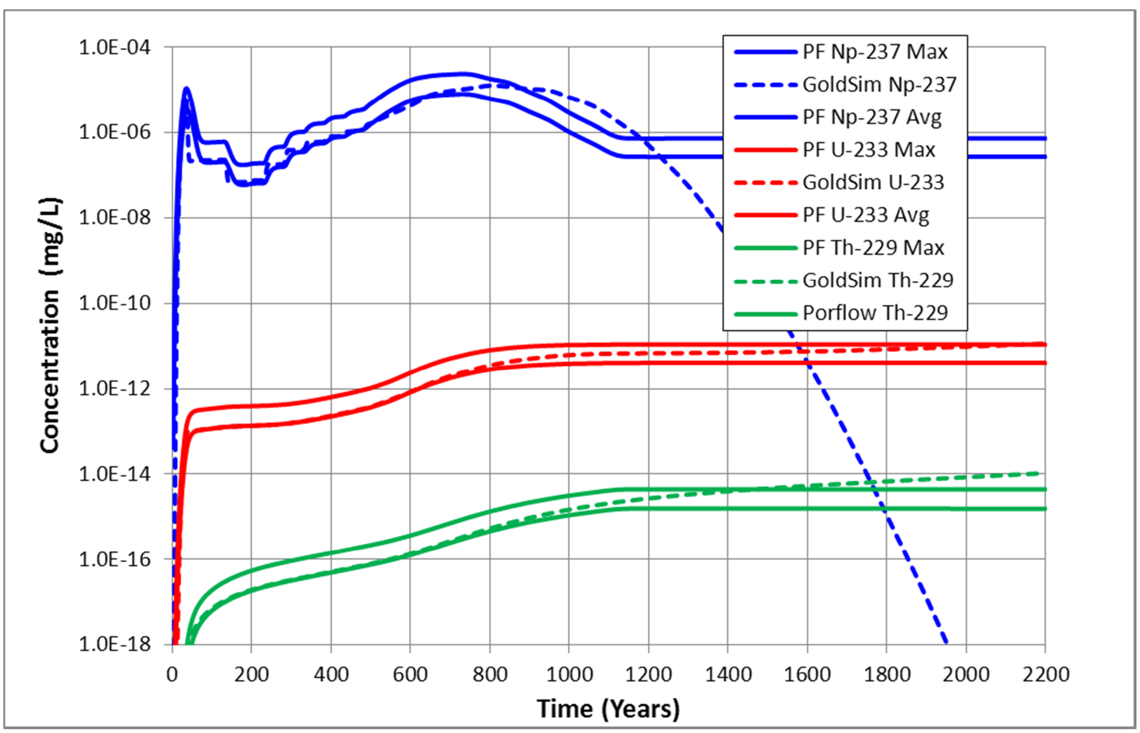

Figure 3-24. Case01 Compliance Point Comparisons for ^{237}Np Family

4.0 Conclusions

Benchmarking exercises were performed to test the updated ELLWF GoldSim trench models and to determine if these models, when utilized in deterministic mode, could produce results similar to the 2008 PA PORFLOW trench models to justify proceeding with the probabilistic sensitivity and uncertainty analyses. The benchmarking consisted of first establishing that the two codes implemented contaminant transport mechanisms accurately before proceeding on to demonstrate that the updated 1D models could produce deterministic results sufficiently similar to the 2D unsaturated zone and 3D saturated zone PORFLOW models developed in the 2008 PA.

4.1 Code-to-Code Conclusions

The code-to-code comparison of GoldSim with PORFLOW was undertaken using an identically configured model domain, material properties and boundary conditions built into each model. The main difference in the codes is that PORFLOW computes water flux terms while GoldSim does not. Therefore, the GoldSim models had water flux terms prescribed that were identical to those computed in PORFLOW. Beyond this, the mechanisms of radioactive decay, partitioning of contaminants between solid and fluid, implementation of specific boundary conditions and the imposition of solubility controls were all tested. The results of the comparison indicate that highly similar results were obtained from both codes. It was also noted that GoldSim has an advantage over PORFLOW in that it simulates all radionuclides simultaneously – thus avoiding a potential problem as demonstrated in the Section 2.6 solubility constrained Case Study. Finally, it is concluded that the use of GoldSim to develop 1D equivalent models to the PORFLOW multi-dimensional models is justified.

4.2 2D/3D to 1D Equivalent Model Conclusions

Benchmarking shows that the 1D GoldSim model can adequately represent the multi-dimensional PORFLOW models. As always, during the benchmarking exercise insight was gained for both models and the system behavior, resulting in additional improvements being made to the ELLWF trench models and providing additional insights into the physical system behavior.

It should be noted that the benchmarking of a Slit Trench is fairly simple because the flow field is essentially one dimensional. However, when engineered barriers are applied to a disposal facility, the flow fields become more complicated and some of the simplifying assumption made for this analysis may not apply. Additionally, based on insight gained during this part of the benchmarking effort, it is recommended that the future PORFLOW models be subjected to both a domain discretization and a time-step sensitivity analysis.

The 2008 PORFLOW 2D Engineered Trench and Slit Trench UZ models have essentially identical vertical dimensions (e.g., initial and final waste zone thickness and distance to the water table), material properties, closure system design, and event chronology (e.g., time of operation, institutional control and final closure). Distance to the 100-m compliance point boundary and groundwater flow path in the 3D SZ model are also similar. These similarities result in nearly identical ET and ST PORFLOW-based disposal limits in the 2008 PA. Thus, it is expected that these two disposal units would exhibit very similar contaminant release and transport behavior when modeled in GoldSim.

Based on the ability of the GoldSim 1D trench models to produce mass flux and concentration curves that are sufficiently similar to 3D PORFLOW ST models for all of the evaluated radionuclides and their progeny, and the aforementioned similarities between Slit and Engineered Trenches, it is concluded that the use of the GoldSim 1D equivalent Slit and Engineered Trench models for further probabilistic sensitivity and uncertainty analysis of ELLWF trench units is justified. Benchmarking of the new ET GoldSim model would be advisable to help ensure that the ET conceptual model has been correctly implemented in GoldSim.

Due to the presence of a grout envelope around cement-encapsulated waste forms in the CIG Trench units, the groundwater flow through the waste zone has a significant lateral component (i.e, 2D flow). The resulting radionuclide release and transport through the waste zone is expected to be substantially different from ET's and ST's during the 300-year period when the grout is assumed to remain intact. Structural stability of this barrier has been assured for at least 300 years by the installation of a reinforced concrete mat or by filling interior void spaces with grout, thus supporting the overlying closure cap. Once this grout barrier degrades and collapses it affects the integrity of the final ELLWF closure cap resulting in increased infiltration (grout barrier assumes properties of the overlying soil in the model after 300 years). After this event, the UZ flow field for the CIG Trench units approaches that of Slit and Engineered Trenches. Because of the presence of these intact barriers and different event timeline, benchmarking is needed to ensure that CIG Trench units are effectively modeled by the revised GoldSim 1D model. With this caveat, the probabilistic sensitivity and uncertainty analysis (Tauxe et al., 2010) was extended to CIG Trenches only for comparison purposes with the other two ELLWF trench types.

5.0 References

ACRI (Analytical & Computational Research, Inc.), 2007. PORFLOW Version 5.97, Analytical and Computational Research, Inc., Los Angeles, CA.

ACRI (Analytical & Computational Research, Inc.). 2008. PORFLOW Version 6.10.3. Analytical and Computational Research, Inc., Los Angeles, CA.

Aleman, 2007. Sebastian Aleman, *PORFLOW Testing and Verification Document*, WSRC-STI-2007-00150, Revision 0, Westinghouse Savannah River Company. Aiken, SC, June 2007.

DOE (U.S. Department of Energy) 1999. *Radioactive Waste Management Manual*, DOE M 435.1, DOE Office of Environmental Management, Washington, DC, July 9, 1999.

GTG, 2007. *GoldSim Version 9.60 (SP1 and SP2*). GoldSim Technology Group LLC, Issaquah, WA, Release Dates: April 23, 2007 (SP1) and August 16, 2007 (SP2).

GTG, 2010. GoldSim Version 10.11 (SP3), GoldSim Technology Group LLC, Issaquah, WA, Release Date: July 27, 2010.

LFRG (Low-Level Waste Disposal Facility Federal Review Group), 2008. *Review Team Report for the E-Area Low-Level Waste Facility DOE 435.1 Performance Assessment at the Savannah River Site*, DOE Low-Level Waste Disposal Facility Federal Review Group Review Team, February 4, 2008.

Tauxe and Catlett, 2010. John Tauxe and Katie Catlett, *Notes on Revisions to the SRS ELLWF Trench Models*, Neptune and Company, Inc., Los Alamos, NM, October 7, 2010.

WSRC, 2008. *E-Area Low-Level Waste Facility DOE 435.1 Performance Assessment*, WSRC-STI-2007-00306, Revision 0, Westinghouse Savannah River Company. Aiken, SC, July 2008.

This page is left blank intentionally

Distribution:

R. S. Aylward, 773-42A
B. T. Butcher, 773-43A
D. A. Crowley, 773-43A
G. P. Flach, 773-42A
F. L. Fox, 704-59E
J. C. Griffin, 773-A
L. L. Hamm,703-41A
R. A. Hiergesell, 773-43A
G. K. Humphries, 730-4B
D. I. Kaplan, 773-42A
M. G. Looper, 704-36E
S. L. Marra, 773-A
J. J. Mayer, 773-42A
T. O. Oliver, 773-42A
M. A. Phifer, 773-42A
K. A. Roberts, 773-43A
R. R. Seitz, 773-43A
D. F. Sink, 704-56E
F. G. Smith, III 703-41A
G. A. Taylor, 773-43A
C. Wilson (1 file copy & 1 electronic copy), 773-43A - Rm. 213