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By Washington River Protection Solutions, LLC., PO Box 850, Richland, WA 99352
Contractor For U.S. Department of Energy, Office of River Protection, under Contract DE-AC27-08RV14800

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Sep 01, 2020
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WMA A-AX Performance Assessment Uncertainty Calculation

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This calculation report is being referenced by the preliminary Waste Management A-AX Performance Assessment (PA), which will be provided to Ecology later this year. In preparation for providing the preliminary PA to Ecology, the documents that support the PA are also be cleared for public release. The analysis was completed in June 2019, but finalization of the document was put on hold until DOE's Low-Level Waste Disposal Facility Federal Review Group (LFRG) reviewed the PA. That review completed last month so finalization of this report is now moving forward.

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Revision 0

WMA A/AX Performance Assessment Uncertainty Calculation

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ENVIRONMENTAL MODEL CALCULATION COVER PAGE

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Date: 5/29/2019

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Software Installation and Checkout Certified:

Integration Lead (Name/Position)	Signature	Date
see attachment 1		

Section 5: Document Review & Approval

	Signature	Date
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Wei Zhou / Engineer (Checker (Name/Position))		6/12/19
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EXECUTIVE SUMMARY

DOE O 435.1, *Radioactive Waste Management* dictates that the U.S. Department of Energy (DOE) radioactive waste management activities shall protect the public from exposure to radiation from radioactive materials, protect the environment, and comply with applicable Federal, State, and local laws and regulations, and to any applicable Executive Orders and other DOE directives. The Performance Assessment provides calculations, including various modeling activities, to assess whether there is reasonable expectation that the facility will provide the necessary levels of protection. DOE M 435.1-1, *Radioactive Waste Management Manual* identifies specific performance objectives, as well as other performance-related factors, considered in the Performance Assessment.

Evaluating whether the residual inventory left behind in a closed waste management area will comply with DOE requirements was performed using a Performance Assessment system model. The system model is one of the modeling tools that was used to evaluate the various prescribed performance objectives identified in DOE M 435.1-1, namely the dose to humans from exposure to contaminated groundwater withdrawn from a water well placed 100 meters downgradient of the closed facility. The system model also evaluates impacts to groundwater resources from dangerous chemicals released from tank and ancillary equipment. One of the primary goals of the system model is to evaluate the uncertainty in calculated human dose at the point of compliance due to uncertainty in input parameters and in recognition of environmental processes that are inherently uncertain. Importance analysis is undertaken to understand which uncertain factors (parameters or processes) exert the greatest influence on the observed range in the model results. The objective of the uncertainty analysis is to support the determination that there is a reasonable expectation of meeting the performance objectives.

The purpose of this environmental model calculation file is to perform an uncertainty and importance analysis using the Waste Management Area A-AX Performance Assessment system model for all pathway impacts. Understanding model and parameter uncertainty is important to building confidence in the model results and identifying when additional research to reduce uncertainty in parameter estimates may be necessary. Uncertainty analysis considers the lack of confidence in predictions of a model due to uncertainties in model parameters or the importance of the features, events, and processes captured in the structure of the model itself. Importance analysis considers the responsiveness of model predictions to selected perturbations of the model's parameters.

The system model was modified to include uncertainties for several parameters. Parameters that were updated to include uncertainty are:

- the net infiltration rate under an intact and degraded surface barrier,
- the effective diffusivity for calculating diffusive releases from the closed waste tanks,
- the contaminant distribution coefficients for cementitious materials (e.g., grout),
- the contaminant distribution coefficients for natural soils,
- the uranium solubility in the pore water contacting the residual waste, and
- the hydraulic conductivity of the saturated zone sediments.

Analyses with the modified system model were performed for 100, 300, 500, and 1,000 Monte Carlo realizations to ensure stability of the simulated results. Latin Hypercube Sampling was invoked to reduce the number of realizations needed to ensure that a stable mean was calculated.

The results reveal that the maximum peak dose in any realization is about 1×10^{-6} mrem/yr during the first 1,000 years after closure. After this time up to 10,000 years the maximum peak dose is 3.6 mrem/yr. The 95% confidence interval for the mean of the peak doses stabilized after 100 Monte Carlo realizations between 0.34 and 0.41 mrem/yr. These peak dose numbers are well below the DOE performance objective of 25 mrem/yr for the All-Pathways dose. A separate calculation (reported elsewhere) concluded that the dose contribution through the air pathway would be even lower than the dose from the groundwater pathway. Therefore, it is highly unlikely that the releases from the residual inventory left in Waste Management Area A-AX would cause a dose to a member of the public to exceed DOE performance objectives in the future.

The timing of the peak dose depended on the uncertainties that determined the radionuclide that contributed the most to the peak. Radionuclide release models with different parameters cause either technetium or uranium to be the dominant dose contributors. When technetium is the dominant dose contributor, the peak dose can occur as early as 2,000 years after closure, but is more likely to be closer to 5,000 years after closure. When uranium is the dose driver the peak is closer to 10,000 years. The later peak for uranium compared to technetium is a result of greater retardation in the natural system below the waste management area.

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LIST OF TERMS, ACRONYMS, AND ABBREVIATIONS

CHPRC	CH2M HILL Plateau Remediation Company
CCUg	Cold Creek unit gravel
CCUz	Cold Creek unit silt
DOE	U.S. Department of Energy
EMCF	Environmental Model Calculation File
EMMA	Environmental Model Management Archive
H1	Hanford formation unit 1
H2	Hanford formation unit 2
H3	Hanford formation unit 3
HISI	Hanford Information System Inventory
IDF	Integrated Disposal Facility
MPR	Model Package Report
NCRP	National Council on Radiation Protection and Measurements
PA	Performance Assessment
PUREX	Plutonium Uranium Extraction (Plant)
SST	Single-Shell Tank
WMA	waste management area
WRPS	Washington River Protection Solutions, LLC

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1.0 PURPOSE

DOE O 435.1, *Radioactive Waste Management* dictates that the U.S. Department of Energy (DOE) radioactive waste management activities shall protect the public from exposure to radiation from radioactive materials, protect the environment, and comply with applicable Federal, State, and local laws and regulations, and to any applicable Executive Orders and other DOE directives. The Performance Assessment (PA) provides calculations, including various modeling activities, used to assess whether there is reasonable expectation that the facility will provide the necessary levels of protection. DOE M 435.1-1, *Radioactive Waste Management Manual* identifies specific performance objectives, as well as other performance-related factors, that need to be considered in the PA.

The objective of developing a system model is to provide one of the modeling tools that will be used to evaluate the various prescribed performance objectives identified in DOE M 435.1-1, namely the dose to humans from exposure to contaminated groundwater. The system model also evaluates impacts to groundwater resources from dangerous chemicals released from tank and ancillary equipment. One of the primary goals of the system model is to evaluate the uncertainty in calculated human dose at the point of compliance due to uncertainty in input parameters and in recognition of environmental processes that are inherently uncertain. Importance analysis is undertaken to understand which uncertain factors (parameters or processes) exert the greatest influence on the observed range in the model results. The objective of the uncertainty analysis is to support the determination that there is a reasonable expectation of meeting the performance objectives.

The uncertainty assessment needs to match the needs of the phase of the safety assessment to which it is applied. First, the magnitude of the projected dose needs to be known, and needs to be compared to the performance objective. Second, the credibility of that output needs to be established. Because of the limited amount of data to support PAs, projected doses will be uncertain. Consequently, the key issue is to identify the conditions for which uncertainty in assumptions or parameters can result in an altered decision. If the decision can be demonstrated to be insensitive to judgments about uncertainty in scenarios, conceptual models, and parameter values, the decision can be defended with confidence. Consequently, the approach to be used for the PA is to consider a range of credible scenarios, conceptual models and combinations of parameter values and determine if any credible combinations could result in a decision of non-compliance.

The purpose of this environmental model calculation file (EMCF) is to use the Waste Management Area (WMA) A-AX PA system model for all pathway impacts to perform an uncertainty and importance analysis. Understanding model and parameter uncertainty is important to building confidence in the model results and identifying when additional research to reduce uncertainty in parameter estimates may be necessary. Uncertainty analysis considers the lack of confidence in predictions of a model due to uncertainties in model parameters or the importance of the features, events, and processes captured in the structure of the model itself. Importance analysis considers the responsiveness of model predictions to selected perturbations of the model's parameters.

Development of the WMA A-AX PA system model is documented in RPP-RPT-60885, *Model Package Report System Model for the WMA A-AX Performance Assessment*. The WMA A-AX PA uncertainty and importance analysis performs the probabilistic analyses using the uncertain inputs documented in this report. Any additional changes necessary to perform the uncertainty analysis are also described in this EMCF.

1.1 OBJECTIVE

The objective of this calculation is exercise the WMA A-AX PA system model in a probabilistic mode and perform an importance analysis to determine the input parameters that have the greatest impact on the observed range of the calculated metrics. The calculated metric is the potential dose to a future member of the public that resides near the closed tanks, and uses/consumes water contaminated by the releases from the tanks and ancillary equipment.

1.2 SUPPORTING DOCUMENTS

The calculations described in this EMCF use conceptual models and mathematical models that are appropriate for the intended use as documented in a series of data package reports, model package reports (MPRs), other environmental calculation reports, and/or other technical literature.

1.2.1 Data Package Reports

Data package reports are reports that are developed for use in the environmental model. Data package reports supporting this calculation support:

X	Conceptual Model Selection	X	Key Assumptions
	Mathematical Model Selection		Model Limitations
	Software Selection	X	Parameterization
	Model Implementation		Other

The data package report(s) that support this calculation is/are:

RPP-RPT-58693	Engineered System Data Package for Waste Management Area A-AX, Revision 0
RPP-ENV-58813	Exposure Scenarios for Risk and Performance Assessments in Tank Farms at the Hanford Site, Washington, Revision 1

In addition, Appendix A provides a discussion for the treatment of uncertainty in PA models and then develops the uncertainty distributions used in this analysis.

1.2.2 Model Package Reports

Model package reports are reports that describe the conceptual and mathematical models used in the calculation. Model package reports supporting this calculation support:

X	Conceptual Model Selection		Key Assumptions
X	Mathematical Model Selection	X	Model Limitations
X	Software Selection	X	Parameterization
X	Model Implementation		Other

The MPR that supports this calculation is:

RPP-RPT-60885 Model Package Report System Model for the WMA A-AX Performance Assessment, Revision 0

1.2.3 Other Environmental Model Calculation Files

Environmental model calculation reports are other calculation reports that develop input or models used in this calculation report and describe the conceptual and mathematical models used in the calculation. Other environmental model calculation reports supporting this calculation support:

	Conceptual Model Selection		Key Assumptions
	Mathematical Model Selection		Model Limitations
	Software Selection	X	Parameterization
	Model Implementation	X	Other

The other EMCF that supports this calculation is the dose calculation without uncertainty:

RPP-CALC-62538 WMA A-AX Performance Assessment Groundwater Pathway Dose Calculation, Revision 0

1.2.4 Other Technical Reports

Other technical reports are reports that provide justification for the analysis approach; specific features, events, or processes to be included or excluded in the conceptual and mathematical models used in the calculation; or justification for model parameter values. Other technical reports supporting this calculation support:

	Conceptual Model Selection	X	Key Assumptions
	Mathematical Model Selection		Model Limitations
	Software Selection	X	Parameterization
	Model Implementation	X	Other

The other technical reports that support this calculation are:

DOE-STD-5002-2017	Disposal Authorization Statement and Tank Closure Documentation
RPP-ENV-58782	Performance Assessment of Waste Management Area C, Hanford Site, Washington
NCRP[1] Report No. 152	Performance Assessment of Near-Surface Facilities for Disposal of Low-Level Radioactive Waste

1.3 DOCUMENT STRUCTURE

The structure of this environmental calculation report follows the required structure of an EMCF.

- Section 2.0 provides supplemental background for the calculation.
- Section 3.0 describes calculation methodology.
- Section 4.0 describes the assumptions and inputs.
- Section 5.0 describes the computational software.
- Section 6.0 describes the output(s) from the environmental model.
- Section 7.0 provides the calculation results and conclusions.
- Section 8.0 is a list of references referred to in this calculation report.

[1] NCRP is the National Council on Radiation Protection and Measurements.

2.0 BACKGROUND

A PA of Single-Shell Tank (SST) WMA A-AX located at DOE's Hanford Site in southeastern Washington is being conducted to satisfy the requirements of the *Hanford Federal Facility Agreement and Consent Order* (Ecology et al. 1989), as well as other Federal requirements and State-approved closure plans and permits. The WMA A-AX PA assesses the fate, transport, and impacts of radionuclides and hazardous chemicals within residual wastes left in tanks and ancillary equipment and facilities in their assumed closed configuration and the subsequent potential doses to humans in the future.

The PA has been structured around the complementary use of process-level and system-level models. Process-level models are those that represent a detailed phenomenological representation of processes of concern in the PA. Process models typically only represent one or a few of the components of the PA, such as groundwater flow and transport, and must be integrated with other modeling elements to perform PA calculations. System-level models are those that are abstracted from the process models, retaining the essential features of the process model, while allowing integration of all aspects of the PA in a single modeling framework. System-level models are often characterized by coarser numerical discretization, lower dimensionality, or other similar simplifications compared to the process-level model.

The system-level model has been developed to assess the long-term performance of WMA A-AX following closure. It has been constructed in order to evaluate the impact of features, processes, and events that are deemed to be relevant at both the spatial and temporal scale of the analysis on release of contaminants from the residual waste, their transport through the geosphere, and eventual dose to humans at the point of compliance.

The system-level model integrates several necessary computational components that allow it to not only mimic the process-level model of the groundwater release pathway, but also to perform several other calculations required for a PA. Computational capability with the WMA A-AX PA system-level model include: (a) waste form degradation and release from various residual inventory-containing sources at closure (tanks and ancillary equipment); (b) flow and transport of contaminants through the vadose zone and saturated zone using an abstracted version of the Subsurface Transport Over Multiple Phases (STOMP)[2] process model; and (c) effective dose and risk from exposure of radionuclides and chemicals at the assessment point for various exposure scenarios.

The system-level model has been developed to be complementary to the more detailed process-level models of the groundwater system. The use of these complementary modeling approaches supports the credibility of both by allowing results to be compared, as demonstrated in RPP-RPT-60885.

2.1 HISTORY

WMA A-AX comprises the 241-A and 241-AX Tank Farms and is located within in the 200 East Area of the Central Plateau of the Hanford Site. The 241-A Tank Farm (A Farm) and

[2] Subsurface Transport Over Multiple Phases (STOMP) is developed and distributed by Battelle Memorial Institute.

241-AX Tank Farm (AX Farm) were constructed between 1953 and 1955 and between 1963 and 1965, respectively. The WMA A-AX tank farms are surrounded by several other double-shell tank farms within the A Complex, and SST Farm 241-C (C Farm) is located nearby to the northwest. WMA A-AX includes catch tanks, diversion boxes, valve pits, pipelines, French drains and unplanned release sites. Numerous liquid discharge facilities used nearby at various times (cribs, trenches, ditches, septic systems, etc.) surround the WMA.

The tanks in both A Farm and AX Farm were designed for the storage of boiling waste generated from irradiated fuel reprocessing at the 202-A Plutonium Uranium Extraction (PUREX) Plant. A Farm contains six 75-ft diameter nominally 1,000,000-gal capacity SSTs that consist of a carbon steel liner inside a concrete tank. AX Farm contains four such SSTs of a later design. A Farm and AX Farm were placed in service in 1955 and 1965, respectively, and both were used to store and transfer waste until mid-1980.

Plans for the future closure of A Farm and AX Farm call for retrieval of wastes remaining in the SSTs (mostly sludge and saltcake solids) to the maximum extent practicable, grouting the residual wastes and interior volume of the SSTs, and construction of a surficial barrier over the tank farms. The WMA A-AX PA uses numerical models to evaluate the ability of the closed WMA to contain the residual waste and prevent unacceptable human exposures due to release and migration of contaminants for at least a period of 1,000 years. The WMA A-AX PA system model uses a probabilistic framework to evaluate the long-term fate of residual waste that is left in the tanks after they are closed and covered by an engineered surface barrier.

2.2 JUSTIFICATION OF METHODOLOGY

One of the major benefits of utilizing a system-level model is that all of the component-level models are integrated into a common modeling framework. The use of a common framework fosters consistency in modeling approaches and ensures that interfaces between the components are implemented in an internally-consistent manner. The result is a single model developed to evaluate the long-term performance of the total system.

One of the principal uses of the system-level model is to evaluate the uncertainty in the performance of the WMA A-AX system. A sensitivity and uncertainty analysis is one of the principle analyses specified in DOE-STD-5002-2017. The complexity and computational burden associated with the different process-level models precludes such an approach for conducting uncertainty analyses. The system-level model has been developed in software code GoldSim©[3] to perform a probabilistic assessment of the impact from residual wastes inside closed tanks at WMA A-AX. Implementation in an efficient, probabilistic model allows for a rigorous assessment of the uncertainty that is inherent in the underlying inputs to the model.

[3] GoldSim© simulation software is copyrighted by GoldSim Technology Group LLC of Issaquah, Washington (see http://www.goldsim.com).

3.0 METHODOLOGY

The approach to the uncertainty and importance evaluation is to use the system model for the WMA A-AX PA, which is described in RPP-RPT-60885, to perform the Monte Carlo dose calculations and supplemental statistical software to post-process the results. The only modifications to the system model are those necessary to update a value or range of values that are part of the uncertainty evaluation and output calculated values for post-processing.

3.1 SELECTION OF TECHNICAL STAFF

The responsible manager or a selected delegate is responsible for selecting the technical staff that develops the conceptual and mathematical approach, performs and documents the calculations, checks the work, and reviews the calculation for technical accuracy and completeness.

X	For the calculations described in this environmental calculation report, the Washington River Protection Solutions, LLC (WRPS) technical lead, as delegated by the responsible manager, has selected the technical staff.
	For the calculations described in this environmental calculation report, the INTERA, Inc. modeling team lead, as delegated by the responsible manager, has selected the technical staff.

3.1.1 Originators

The originators or preparers of the environmental model calculation develop the methodology; gain early concurrence with the senior reviewers; identify project conditions, assumptions, and inputs; and prepare the calculation and associated calculation report.

3.1.1.1 Kearn Patrick Lee (Pat) (ORANO Federal Services, LLC)

Advisory Engineer
M.C.E., 1996, Civil and Environmental Engineering, University of Delaware
B.Ch.E., 1993, Chemical Engineering, University of Delaware

Pat Lee has over 18 years of modeling experience using the GoldSim© Radionuclide Transport Module to conduct PAs for DOE. He was a lead analyst on the high-level waste PA for Yucca Mountain from 2001 to 2010 and has been the technical lead for the Integrated Disposal Facility (IDF) PA since 2015. He has presented models he developed for the Yucca Mountain Project at several GoldSim© user's conferences and he also developed Yucca Mountain Project training modules to provide an overview of the Yucca Mountain high-level waste PA model. He has completed all reading assignments that are procedurally required to perform environmental fate and transport calculations. He has developed and checked several other models for the IDF PA. He is also familiar with the statistical techniques used to evaluate parameter importance in Monte Carlo analyses.

3.1.1.2 Glenn Taylor (WRPS / TerraGraphics, Inc.)

Glenn Taylor is a second originator of this work. Glenn has more than 20 years of engineering experience, the last 12 of which has been in a Performance Assessment group performing the type of work that was performed for this calculation report. Glenn's extensive experience in developing and reviewing GoldSim© (and other software) models and applying statistical methods to evaluate model results makes him an ideal choice for this role on this EMCF.

3.1.2 Checkers

The checker reviews the environmental model calculation to verify that it is clearly developed and that the calculation was performed as described and without error. Checking includes ensuring that all the inputs are consistent with the original referenced material. The checker documents the review of the calculation on an appropriate Checker Log.

Wei Zhou (INTERA, Inc.)
Senior Engineer
Ph.D., 1992, Nuclear Engineering, University of California at Berkeley
M.S., 1986, Mechanical Engineering, San Jose State University
B.S., 1982, Mechanical Engineering, Beijing University of Technology

Wei Zhou has more than 30 years of experience in the areas of performance and safety assessment of near-surface and deep geological radioactive waste repositories, risk assessments for organic wastes including dense and light non-aqueous phase liquids and volatile organic compounds, and the geological sequestration of carbon dioxide (CO_2). She has provided technical support in these areas to industrial, governmental, and international organizations such as the Electric Power Research Institute, International Atomic Energy Agency (IAEA), Nuclear Energy Institute, Korean Hydro and Nuclear Power, Canadian Petroleum Technology Research Institute, U.S. Environmental Protection Agency, DOE, Swedish Nuclear Inspectorate, Japan Atomic Energy Agency, Taiwan Institute of Nuclear Energy Research, International Energy Agency, Nuclear Energy Agency, and the Commission for European Communities. She specializes in modeling and simulation of radionuclide transport, coupled heat and mass transfer in fractured media, as well as multiphase and multi-component transport systems using public or commercial codes including TOUGH2[4], TOUGHREACT[5], STOMP, ECLIPSE suite codes, MATLAB®[6], and GoldSim©. Her expertise also includes developing customized software using FORTRAN and C++. She has completed all reading assignments that are procedurally required to perform environmental fate and transport calculations.

[4] TOUGH2 software was developed by Lawrence Berkeley National Laboratory, University of California, Berkeley, California with support from the Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division of the U.S. Department of Energy.
[5] TOUGHREACT software was developed by Lawrence Berkeley National Laboratory, University of California, Berkeley, California with support from the Office of Science, Office of Geothermal Technologies of the U.S. Department of Energy.
[6] MATLAB® (matrix laboratory) is a registered trademark of The MathWorks, Inc., Natick, Massachusetts.

Wei was the lead checker for this work and reviewed the GoldSim© model, verifying that inputs in the model matched the source documents, the model was implemented correctly for the intended purpose, and that the outputs were exported correctly.

3.1.3 Senior Reviewers

The senior reviewer(s) reviews the calculation methodology, assumptions, and criteria and verifies that they are appropriate for the intended use and that the calculation was developed correctly.

Matthew W. Kozak (INTERA, Inc.)
Ph.D., 1988, Chemical Engineering, University of Washington
B.S., 1981, Chemical Engineering, Cleveland State University

Dr. Kozak has more than 27 years of experience in the areas of performance assessment of near-surface and geological radioactive waste repositories, regulatory development, dose assessment for residual contamination of soils and buildings, toxic materials risk assessment, and mixed waste issues. He is the author of over 100 publications on these topics. He has supported national programs in the U.S. and countries in Europe, Asia, and Africa to site, develop, construct, and analyze facilities for disposal of radioactive waste.

He has participated in a number of international research programs, including the IAEA's Coordinated Research Program on Improvement of Safety Assessment Methodologies, and its successor programs: Application of Safety Assessment Methodologies, Practical Illustration and Use of the Safety Case Concept in the Management of Near-Surface Disposal, and most recently Modelling and Data for Radiological Impact Assessments.

He is a principle investigator for the WMA A-AX PA.

3.2 CONCEPTUAL MODEL

The conceptual models for the dose calculations and importance analysis are described by reference to the applicable documentation.

3.2.1 System Model

The conceptual model for the WMA A-AX PA dose calculations is described in RPP-RPT-60885 Section 3.0. The initial effort to develop the system model and uncertainties captured within it are informed by the analyses conducted for the WMA C PA. The WMA C PA has previously been reviewed by DOE Headquarters and is in the process of a formal public review and U.S. Nuclear Regulatory Commission review. WMA C is in the same general vicinity on the Hanford Site as WMA A-AX and consists of similar waste tanks set into a similar geology. WMA C PA analysis results were used to inform the development of the WMA A-AX system model and assign uncertainties to input parameters.

For the calculations performed in the report, the system model was exercised in a Monte Carlo probabilistic mode to generate a range of expected outcomes derived by the uncertainty in the applied input parameters. In the Monte Carlo mode, discrete sets of input parameter values are selected from probability distribution functions, and the model was exercised with the sampled values. A probability distribution function of model output is constructed from all of the different realizations performed in the analysis. Latin Hypercube Sampling was invoked to develop stable mean result with fewer Monte Carlo realizations.

3.2.2 Importance Analysis

As part of the PA development process, an importance analysis was performed to evaluate the parameters in the WMA A-AX PA model that have a significant influence on the dose output. This approach is consistent with the purpose of an importance analysis as described in NCRP Report No. 152, which states that an importance analysis is

> *"… an integration and interpretation of results obtained from the performance assessment process for the purpose of identifying assumptions and parameters which, when changed within credible bounds, can affect a decision about regulatory compliance."*

The WMA A-AX PA is an iterative process. In this first iteration of the PA, the importance analysis is not intended to inform decisions regarding regulatory compliance, but rather inform the data gathering and model refinement process by identifying the uncertainties in the parameters that most significantly affect the results of the PA.

The WMA A-AX system model has 117 stochastic inputs that are used to evaluate parameter uncertainty. An importance analysis was performed to identify which of the uncertain parameters have the greatest influence on the observed range in a calculated result. In other words, the importance analysis identifies which inputs contribute the most uncertainty to the output. Accordingly, the importance analysis also identifies the uncertainty parameters that have very little influence on the uncertainty in the calculated result. A critical aspect of an importance analysis is that it only identifies the importance of model parameters that include uncertainty. Parameters with deterministic values may affect the magnitude of a modeled result but do not affect the uncertainty in the model result. Although a deterministic parameter may be important to quantifying the magnitude of a projected result, it will not be identified as a parameter that is important to quantifying the uncertainty in the projected result.

To complete the discussion, single realization analyses are also performed for selected realizations to demonstrate how parameters identified (and not identified) in the importance analysis affect the groundwater dose results. In a single realization analysis, a result in the uncertainty analysis is explained in relation to the sampled values in that realization.

3.3 MATHEMATICAL MODEL

The mathematical model for the WMA A-AX PA dose calculations is described in RPP-RPT-60885 Section 3.0.

3.4 CALCULATION PROCEDURE

The calculation is initiated by obtaining a copy of the WMA A-AX PA system model from the Environmental Model Management Archive (EMMA) or other designated location (e.g., EMMA staging).

1. OPEN the WMA A-AX PA system model in GoldSim© version 12.0.

2. PERFORM any necessary modifications to the model and document the purpose of these changes.

3. ENSURE a multivariate element is included in the model for each targeted output and VERIFY that the desired output result and all stochastic inputs are included.

4. CONFIRM/UPDATE the model settings (run duration, time step schedule, and number of Monte Carlo realizations).

5. PERFORM the model run.

6. OUTPUT the multivariate result(s) to a tab-delimited text file or spreadsheet.

For the importance analysis, record the importance analysis metrics calculated using the multivariate result elements. A description of the calculated metrics is provided in Section 7.6.

For corroboration of the importance analysis results using stepwise regression techniques using JMP software (see Section 7.6.2.1), copy the multivariate results data table into a JMP workbook and perform the importance analysis using the built-in capabilities of the software.

For corroboration of the importance analysis results using the random forest technique using R software (see Section 7.6.2.2):

1. COPY the R-script used to perform the importance analysis to the same location as the model output file.

2. VERIFY that the input file specified in the R-script matches the filename and location of the GoldSim© results file. UPDATE the name and location of the input file if necessary.

3. START R and run the R-script used to perform the importance analysis.

4. COPY the output of the importance analysis into a spreadsheet application and SORT the output by the Importance Measure metric.

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4.0 ASSUMPTIONS AND INPUTS

This section provides the relevant assumptions and any inputs that are specific to the uncertainty analysis. Key assumptions for the development and implementation of the system model are documented in RPP-RPT-60885.

4.1 KEY ASSUMPTIONS

Key assumptions and modeling decisions for the uncertainty calculations are:

- Releases to the air pathway are neglected in the uncertainty analysis.
- Initial inventories in the tanks and in the ancillary equipment are post-retrieval estimates and are not treated with uncertainty.
- Releases from the residual waste in the tanks are diffusion-controlled; the surface barrier and tank dome limit the flow of water into the tanks for 10,000 years.
- One-dimensional flow and transport models using flow fields developed from and benchmarked against three-dimensional flow and transport simulations are adequate for simulating transport in the natural system below the WMA. Regression models can be used to scale the flow fields, moisture content and Darcy velocity, to account for uncertainty in the recharge rates.
- The lifetime of the surface barrier is not treated with uncertainty in this analysis, uncertainty in the lifetime of the surface barrier is addressed in sensitivity studies.
- Contaminant transport through sediments in the vadose and saturated zone use distribution coefficients for sand with a correction for gravel content. The gravel content is not treated with uncertainty.
- Dose conversion factors are not treated with uncertainty.

4.2 INPUTS

The WMA A-AX system model uncertainty analysis uses both deterministic and uncertain parameters. Deterministic parameters are input parameters that have a fixed value. Using deterministic values for some parameters is not intended to reflect that a particular input is known with certainty. Generally, deterministic values are used when the sensitivity to a particular parameter is known in advance or studied separately. In rare instances, deterministic values are used when there is no technical basis for treating a parameter with uncertainty.

For instance, the correlation between tank inventory and groundwater dose is evaluated separately using a sensitivity analysis. For radionuclides that have linear transport processes (i.e., no solubility limit with linear sorption isotherms), the sensitivity analysis demonstrated that there is a linear correlation between inventory and dose; when the inventory of a radionuclide is doubled, the dose from that source is also doubled. Therefore, the uncertainty analysis does not include uncertainty on inventory. In addition, the groundwater dose model used to convert groundwater concentration to dose is also linear between concentration and dose. Therefore, the uncertainty analysis does not include uncertainty on the exposure scenario parameters. The

uncertainty analysis does not attempt to forecast cyclical changes in climate or changes in human behavior over the next 10,000 years.

The WMA A-AX system model includes 117 parameter distributions. The distribution coefficients for 37 elemental or chemical constituents in sand and silt account for 74 of the 117 parameters. The distribution coefficients in cementitious materials account for another 37 of the 117 parameters. The remaining six distributions are used to evaluate uncertainty in the solubility of uranium, the diffusion coefficient for transport through the tank bottom, the net infiltration rates beneath the intact and degraded surface barriers, the lifetime of the grout used to fill the closed waste tanks, and the hydraulic conductivity of the sediments in the aquifer beneath the WMA.

Appendix A discusses the development of the uncertainty distributions used for these parameters.

5.0 SOFTWARE APPLICATIONS

GoldSim© was the primary software used for system models calculations. It is approved software and the information required is provided in this section. Microsoft Excel®[7] spreadsheets were used to create visual displays presented in Section 7.0 and perform linear regressions.

The software applications used to perform this calculation are approved, managed, and used in compliance with the CH2M HILL Plateau Remediation Company (CHPRC) requirements of PRC-PRO-IRM-309, "Controlled Software Management." CHPRC's software requirements for the GoldSim software also meet WRPS's software requirements.

Two other commercial software packages were used to generate statistical information necessary to understand the model's response to changes in the input parameters. These software applications are registered in HISI. These software packages are JMP[8] version 13.2.1 (HISI # 2744) and R (HISI # 3911). Both software applications are graded Level D or lower and are used for corroboration of results. These two applications were used to corroborate GoldSim importance analysis calculations; the software discussion below is focused on the GoldSim software.

5.1 SOFTWARE IDENTIFICATION

- GoldSim© Pro (with Radionuclide Transport Module)
- Version: 12.0
- Hanford Information System Inventory (HISI) Identification Number: 2461
- System: Dell™ Optiplex™[9] 7050 (WF40244).

5.2 SOFTWARE QUALITY ASSURANCE

Software development of GoldSim© Pro meets ANSI/AMSE NQA-1-2008, *Quality Assurance Requirements for Nuclear Facility Applications* with NQA-1a-2009 Addenda software requirements, as well as the requirements specified under DOE O 414.1D, *Quality Assurance* for Safety Software. The applicable software quality assurance documents are:

- CHPRC-00180, *GoldSim Pro Functional Requirements Document*
- CHPRC-00175, *GoldSim Pro Software Management Plan*
- CHPRC-00256, *GoldSim Pro Requirements Traceability Matrix: Version 12.0*
- CHPRC-00224, *GoldSim Pro Software Test Plan*

[7] Excel® is a registered trademark of Microsoft Corporation in the U.S. and other countries.
[8] JMP is a product of SAS Institute Inc., SAS Campus Drive, Cary, North Carolina.
[9] Dell™ and Optiplex™ are trademarks of Dell Inc., Round Rock, Texas.

- CHPRC-00262, GoldSim Pro Acceptance Test Report: Version 12.0.

5.3 SOFTWARE INSTALLATION AND CHECKOUT

Acceptance and installation tests of the GoldSim© Pro simulation software demonstrate that it is appropriate for its intended uses for the WMA A-AX PA and that it has been successfully installed on the computing systems used to conduct WMA A-AX PA modeling. The software installation and checkout form for GoldSim© Pro is provided in Attachment 1 to this EMCF.

5.4 STATEMENT OF VALID SOFTWARE APPLICATION

GoldSim© Pro is a valid software application and was applied in this report within its range of intended uses for which it was tested and approved. GoldSim© Pro was utilized for DOE to assist in performing simulation of radioactive mass conservation including decay and ingrowth for the Hanford Site.

6.0 CALCULATION

The WMA A-AX PA uncertainty and sensitivity analysis has two principle components, the probabilistic results for selected calculated results and the importance analysis on the peak All-Pathways dose.

6.1 DESCRIPTION OF MODEL CHANGES

There are two primary types of changes made to the WMA A-AX system model documented in the MPR (RPP-RPT-60885). These change types are:

1. Update uncertainty parameter ranges
2. Add result elements to capture model results.

Changes of the first type recognize that many of the distributions included in the model documented in the MPR contained preliminary values derived from previous work at WMA C. These distributions are refined for this WMA A-AX uncertainty analysis.

Changes of the second type are necessary to record and output calculated results needed in the importance analysis.

6.1.1 Model Configuration Control

Model configuration control is enforced through the GoldSim© Version Manager (see Figure 6-1). A version control configuration point was added to the model documented in RPP-RPT-60885 on April 8, 2019. Any changes to the model after this configuration point are tracked by the GoldSim© Version Manager. A report of the model changes can be generated by clicking "Generate Report" in the Version Manager. The report provides a listing of the model elements that have been edited relative to the April 8, 2019 configuration point. After performing all necessary changes to the model to perform the uncertainty analysis, the model run was performed and a new version control point was added to the model. This new control point establishes the basis for additional uncertainty analysis work.

6.1.2 Model Checking

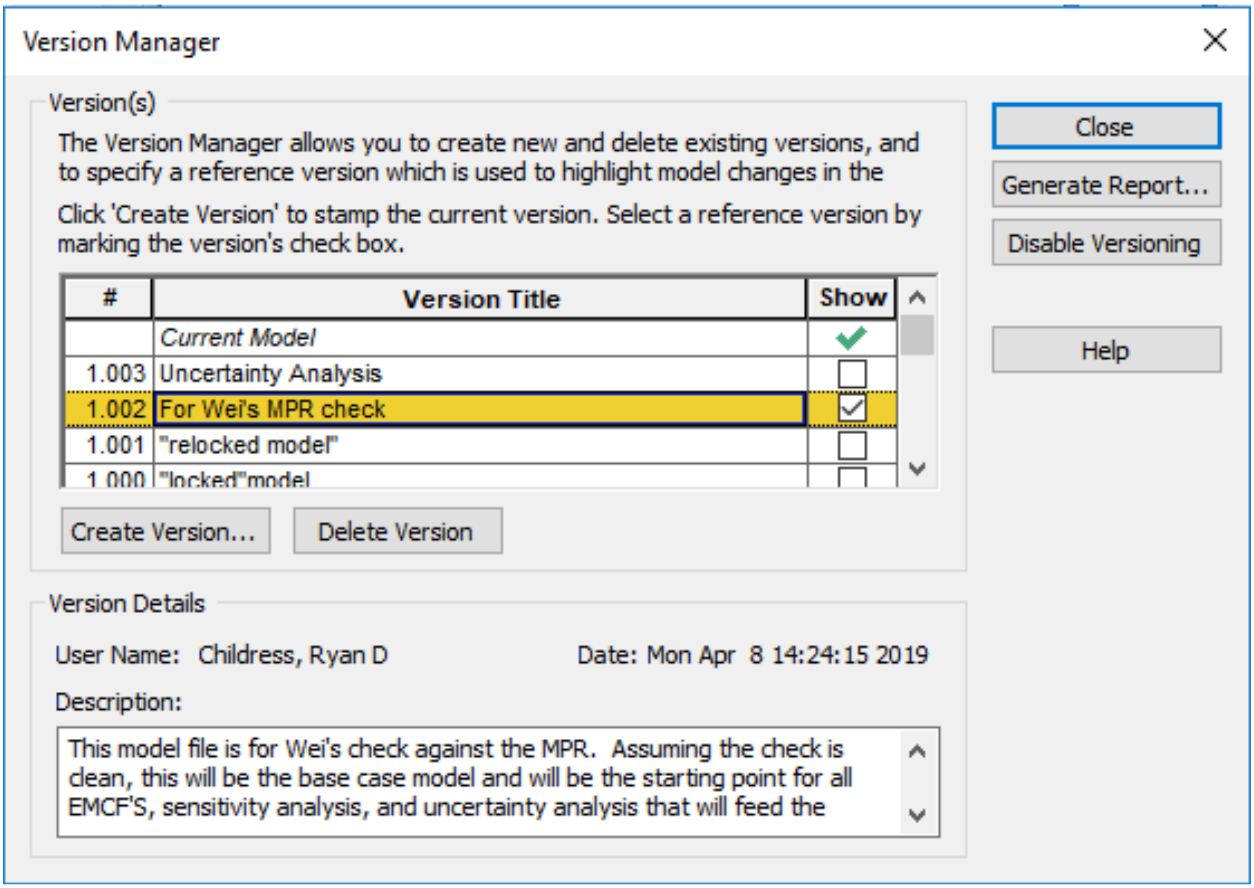
Checking of the WMA A-AX PA system model was performed during model development and is documented in RPP-RPT-60885. Checking of the changes identified in the Version Manager report of changes is a quality assurance check to ensure that the simulation settings are appropriate for the specified case. Checking model changes and simulation settings are performed by an independent modeler. A signed checklist is included in Attachment 2.

6.1.3 Importance Analysis Checking

Checking of the Importance Analysis calculation is performed by an independent checker that is familiar with different methods to test statistical importance. In addition, two alternative

methods were used to corroborate the importance analysis performed using the GoldSim software. Prior to performing the corroboration using the random forest method, an independent checker reviewed the R-script used to perform the calculation. Corroboration of the importance analysis results is documented in Section 7.6.2.

Figure 6-1. System Model Configuration Control Using the Version Manager.



6.2 DESCRIPTION OF CALCULATED OUTPUT

The WMA A-AX PA uncertainty and sensitivity analysis has two principle components, the probabilistic results for selected calculated results and the importance analysis on the peak All-Pathways dose. Unless otherwise noted, dose to a member of the public in the future is evaluated at a location that is 100 meters from the closed tanks in the prevailing groundwater flow direction. Dose contributions from the air pathway are excluded from the All Pathway dose analysis because the air pathway has been screened out.

6.2.1 Selected Dose Results for the All-Pathways Analysis

Probabilistic dose results are reported for different metrics calculated by the WMA A-AX PA system model. The calculated metrics are determined at each timestep in the model so that key results are time histories of calculated results or final values representing peak occurrences in each realization. Time history results are reported for the simulated duration, 10,000 years. Note that model time zero years is equated to the time of closure of the WMA. Unless otherwise specified, the dose results are plotted for all realizations together with the mean dose, 5th-, 50th-, and 95th-percentile doses. Note the percentile plots do not represent a specific percentile sampling of the probability density functions. The 5th-percentile plot is the series of values where 5% of the reported values at each time step are lower than the value plotted. The median, or 50th-percentile plot is the value at each time step that has an equal number of results that are higher and lower than the represented value. The 95th-percentile plot is the series of values where 95% of the reported values at each time step are lower than the value plotted.

The probabilistic results reported in this EMCF include the total groundwater dose from each tank farm in the WMA. Groundwater flow modeling suggests that the plume originating from each farm is expected to have minimal overlap along its point of highest concentration so the dose from each farm is evaluated separately. The total dose is the sum of the doses from all radionuclides reaching the point of calculation from each tank farm. The dose results do not include the air pathway dose because the air pathway analysis has been screened out of the total dose evaluation for the WMA.

6.2.2 Other Selected Results for the All-Pathways Analysis

Results for other calculation metrics include the groundwater pathway dose for key contributors and cumulative releases to the vadose zone and saturated zone for key contributors.

6.2.3 Importance Analysis

The output of the importance analysis is a listing of the uncertain parameters that most significantly affect the uncertainty in a calculated metric (e.g., the peak total dose from each tank farm) as determined by a statistical analysis (e.g., using rank regression or the Random Forest algorithm). The analysis is performed for other metrics in order to improve the understanding of the model's response to varied parameters.

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7.0 RESULTS AND CONCLUSIONS

The uncertainty analysis of the WMA A-AX PA model is discussed in five categories:

1. Stability Analysis (Section 7.1)
2. Total Groundwater Dose Analysis (Section 7.2)
3. Radionuclide Groundwater Dose Analysis (Section 7.3)
4. Cumulative Release to Vadose Zone Analysis (Section 7.4)
5. Cumulative Release to Saturated Zone Analysis (Section 7.5).

Dose analyses present dose results as a function of simulation time and peak values in 10,000 years. Cumulative release analyses present total mass releases from the WMA source terms over the 10,000-year simulation period.

Throughout the discussion, the term total groundwater dose refers to the sum of the doses from individual radionuclides. Total groundwater doses are presented by source and by farm. Total doses by source are presented by tank farm for each waste storage tank in a tank farm and the combined dose from all pipelines and ancillary equipment sources in a tank farm (referred to as "Non-Tank" sources). Unless otherwise indicated, total dose by farm is the combined dose from all sources in a farm (tanks plus pipelines plus ancillary equipment).

Mean and statistical results for a specified metric (e.g., total groundwater dose) are plotted as time histories. In these curves, the mean time history result is the arithmetic mean of all realizations in a simulation at the given time; the mean time history result is not the dose using the mean value from all of the uncertainty distributions. Similarly, the median time history result is the 50th-percentile value at the given times; the median time history result is not the dose using the median value from all of the uncertainty distributions. Analogous histories are also provided for the 5th- and 95th-percentiles of a specified metric.

Two other metrics that are discussed are the "peak of the mean" and the "mean of the peaks." The peak of the mean is the highest value of the mean time history result. The mean of the peaks is the arithmetic average of the highest value in each realization's time history result.

7.1 STABILITY ANALYSIS

In a probabilistic analysis that includes multiple parameters with uncertainty distributions, multiple outcomes of a given metric (e.g., total groundwater dose) will be generated. Selecting an adequate number of realizations to perform for the uncertainty analysis must balance computational run times with the generation of a statistically stable result. The stability analysis demonstrates that the number of samples used in the uncertainty analysis is sufficient to provide a reasonable expectation of the dose result. In the stability analysis, the time history of groundwater doses from each tank farm are compared for different numbers of Monte Carlo simulations. Latin Hypercube Sampling is performed to reduce the number of realizations necessary to have the mean and median dose histories converge on a stable result.

In the statistical stability analysis, the WMA A-AX system model was exercised for 100, 300, 500, and 1,000 Monte Carlo realizations invoking Latin Hypercube Sampling. Statistics for the peak total dose by tank farm for each Monte Carlo realization are shown in Table 7-1. The statistical stability test demonstrates that with 100, 300, 500, or 1,000 realizations, the 95% confidence interval around the mean peak total dose is well below the DOE performance objective of 25 mrem/yr. Furthermore, the confidence interval overlaps after just a few hundred realizations. The 95% confidence interval, assuming the peak total dose is normally distributed, is computed using Equation 7-1.

$$CI_{95} = \bar{x} \pm z^* \frac{\sigma}{\sqrt{n}} \tag{7-1}$$

Where:

CI_{95}	=	95th-percentile confidence interval around the mean
$\bar{x}$	=	mean peak dose value
z^*	=	critical value (= 1.96 for a two-sided 95th-percentile confidence interval)
σ	=	standard deviation
n	=	sample size.

Table 7-1. Statistical Stability of the Peak Mean Dose (mrem/yr).

Dose Case		100 Realizations	300 Realizations	500 Realizations	1,000 Realizations
Total Groundwater Dose (mrem/yr): 241-A Tank Farm					
Peak Dose Range	Minimum	0.015	1.5E-03	2.5E-04	1.7E-06
	Maximum	2.8	3.6	2.9	3.4
Mean Peak Dose		0.40	0.37	0.39	0.38
Standard Deviation		0.39	0.33	0.33	0.33
Median Peak Dose		0.28	0.29	0.28	0.28
95%-Confidence Interval	Lower	0.33	0.34	0.36	0.36
	Upper	0.48	0.41	0.41	0.40
Total Groundwater Dose (mrem/yr): 241-AX Tank Farm					
Peak Dose Range	Minimum	4.5E-04	1.0E-05	1.6E-06	3.2E-09
	Maximum	0.28	0.32	0.45	0.60
Mean Peak Dose		0.058	0.057	0.059	0.058
Standard Deviation		0.044	0.045	0.046	0.047
Median Peak Dose		0.045	0.046	0.045	0.046
95%-Confidence Interval	Lower	0.049	0.052	0.055	0.055
	Upper	0.067	0.063	0.063	0.061

The mean and median values for total groundwater dose from A Farm and AX Farm are plotted for the cases with different numbers of realizations as a function of time in Figure 7-1 to Figure 7-4.

Figure 7-1. Comparison of the Mean Total Groundwater Dose for 100, 300, 500, and 1,000 Realizations: 241-A Tank Farm.

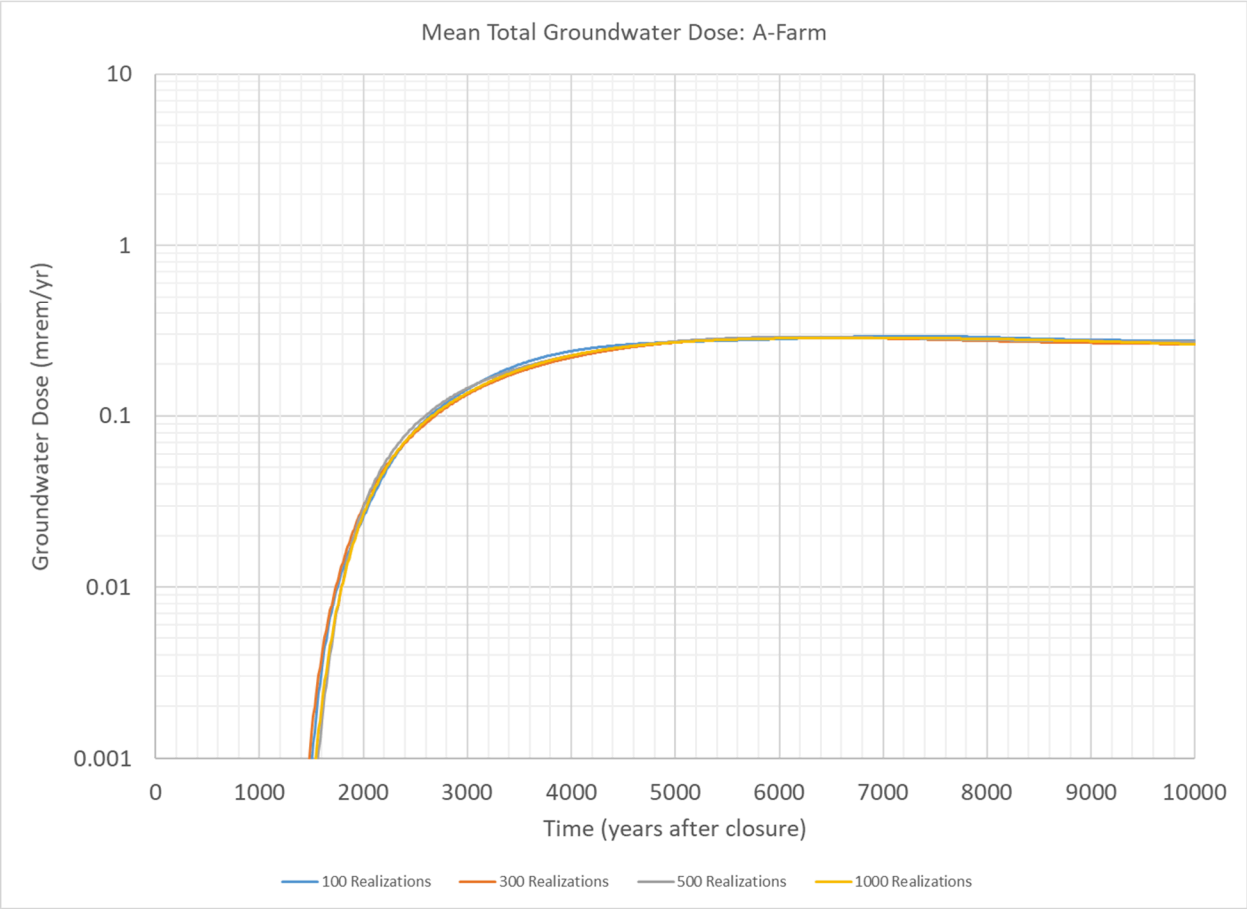


Figure 7-2. Comparison of the Median Total Groundwater Dose for 100, 300, 500, and 1,000 Realizations: 241-A Tank Farm.

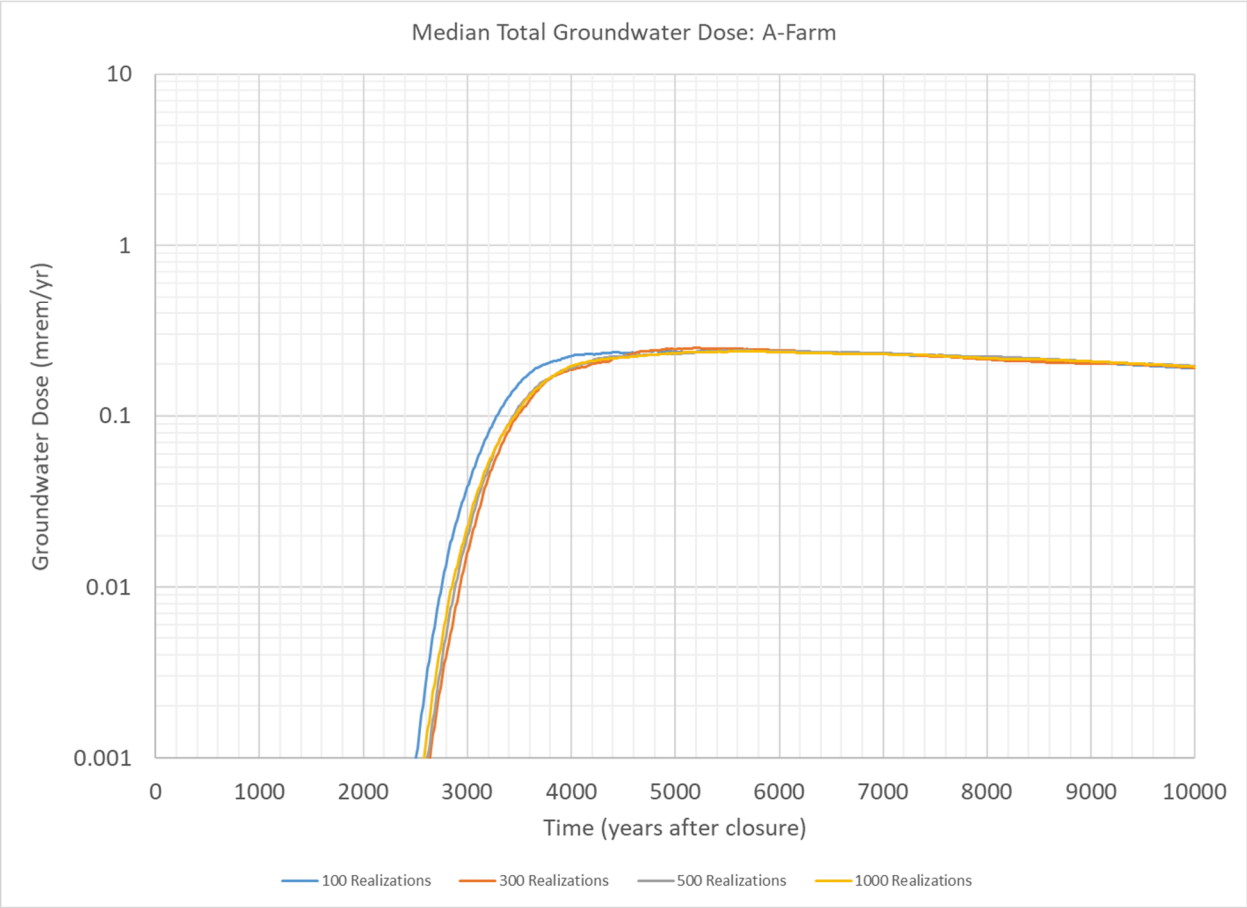


Figure 7-3. Comparison of the Mean Total Groundwater Dose for 100, 300, 500, and 1,000 Realizations: 241-AX Tank Farm.

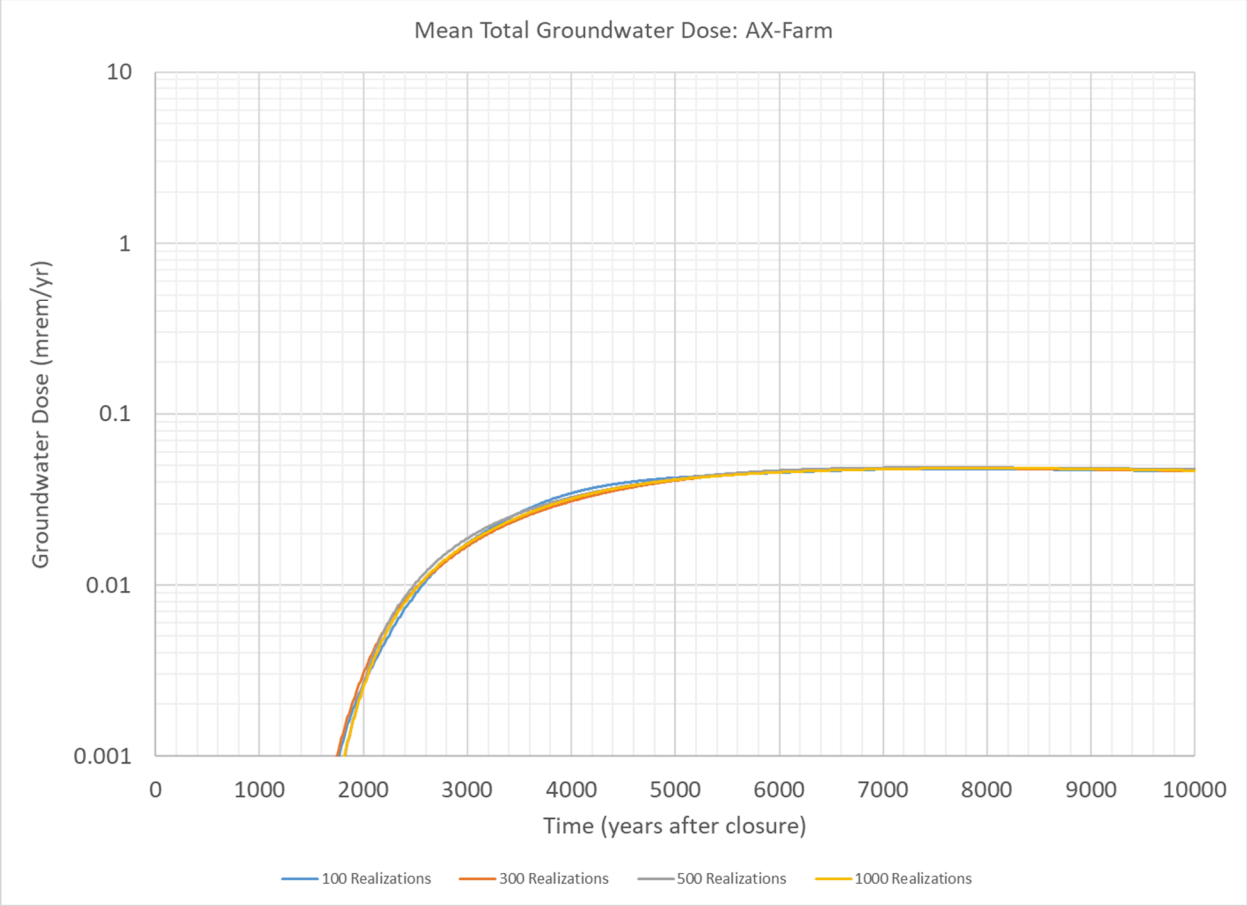
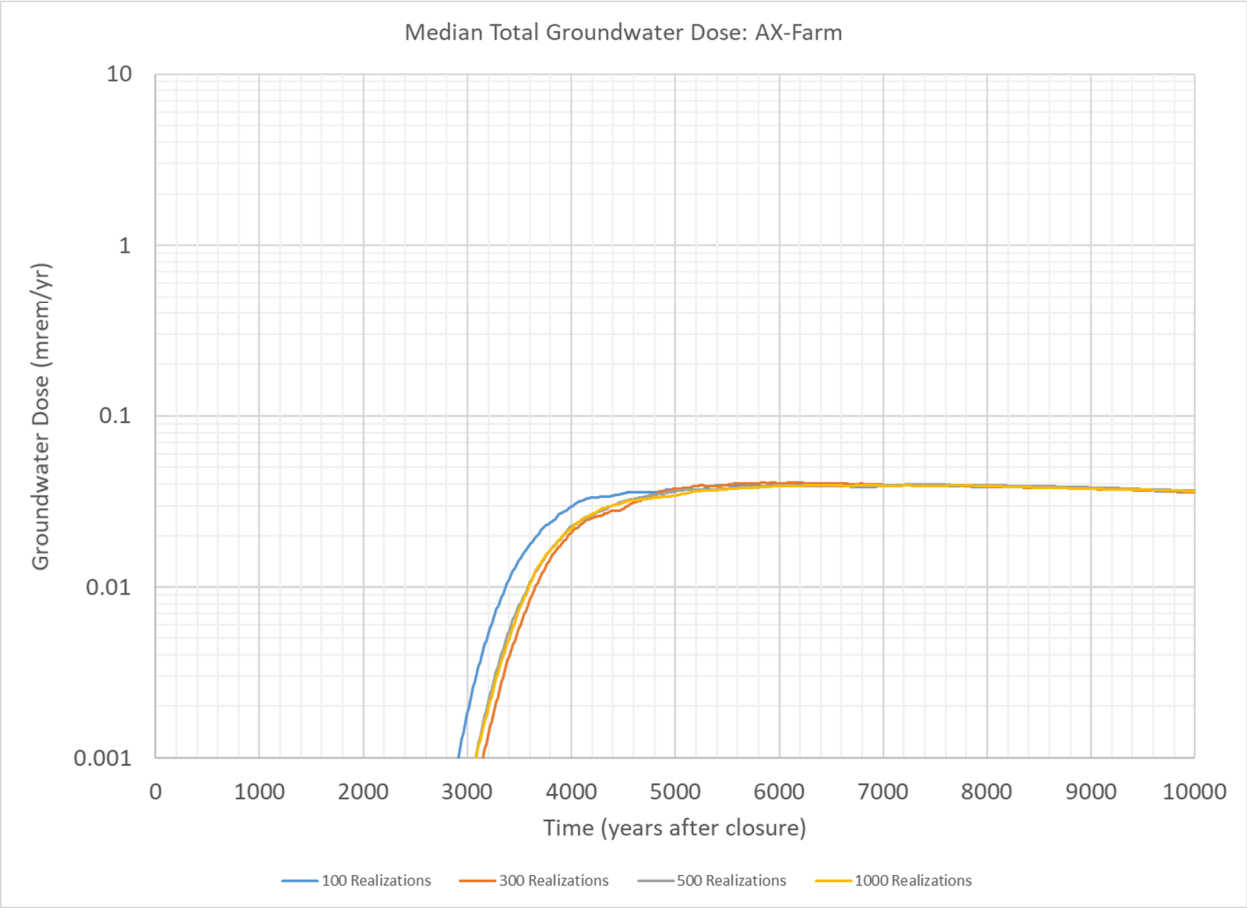


Figure 7-4. Comparison of the Median Total Groundwater Dose for 100, 300, 500, and 1,000 Realizations: 241-AX Tank Farm.



7.2 TOTAL GROUNDWATER DOSE ANALYSIS

The statistical stability study revealed that the 300, 500, and 1,000 realization runs produce similar results. For consistency with other PAs done at the Hanford Site, the uncertainty analysis is focused on the 300 realization run.

The total groundwater dose from all A Farm and AX Farm sources is shown in Figure 7-5. The total groundwater dose statistics from all A Farm and AX Farm sources are compared to the deterministic case with fixed input parameter values in Figure 7-6. A review of the total dose results reveals that no realization has a total groundwater dose that exceeds 1×10^{-6} mrem/yr in the first 1,000 years. Since doses below 1×10^{-6} mrem/yr are well below DOE's performance objective of 25 mrem/yr, the total dose analysis focuses on the total dose in 10,000 years. The purpose of this analysis is not to simply extend the simulation period, but to understand which parameters could shift the timing of the peak dose.

The total groundwater dose from A Farm sources is higher than the total groundwater dose from AX Farm sources. When compared to the deterministic analysis, the breakthrough times in the

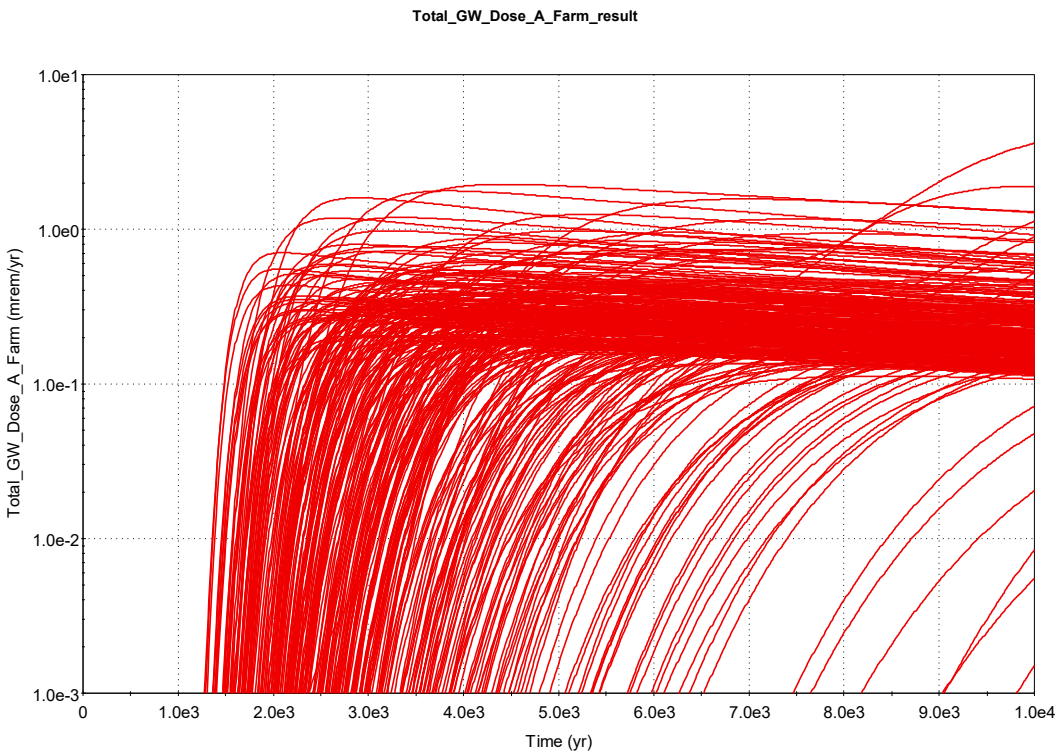
deterministic analysis are most consistent with the breakthrough times at the 95th-percentile of the 300 realizations. However, the magnitude of the dose in the deterministic analysis is most consistent with the magnitude at the 50th-percentile of the 300 realizations.

It is also observed that the mean contributions from the non-tank sources in the two tank farms is high enough to be viewed on the dose scale in Figure 7-7, but that the 95th-percentile almost shows no dose history for these sources. This indicates that just a few realizations (less than 5%) with high dose histories are driving the mean dose result for these sources.

The mean and median total dose from the two tank farms are driven by the dose from two tanks, SSTs 241-A-104 and 241-A-105. These two tanks have the largest inventories. Tank 241-A-105 has a large bulge in the tank bottom and was assumed to be minimally retrieved to limit releases to the vadose zone during retrieval. Figure 7-7 shows the mean total groundwater dose by source. The figure includes the mean time history results for each source together with the equivalent dose from the deterministic analysis that uses fixed parameter values for all inputs. Figure 7-8 through Figure 7-10 show analogous plots for different statistics.

Figure 7-5. Total Groundwater Dose for 300 Realizations: (a) 241-A Tank Farm, (b) 241-AX Tank Farm.

(a)



(b)

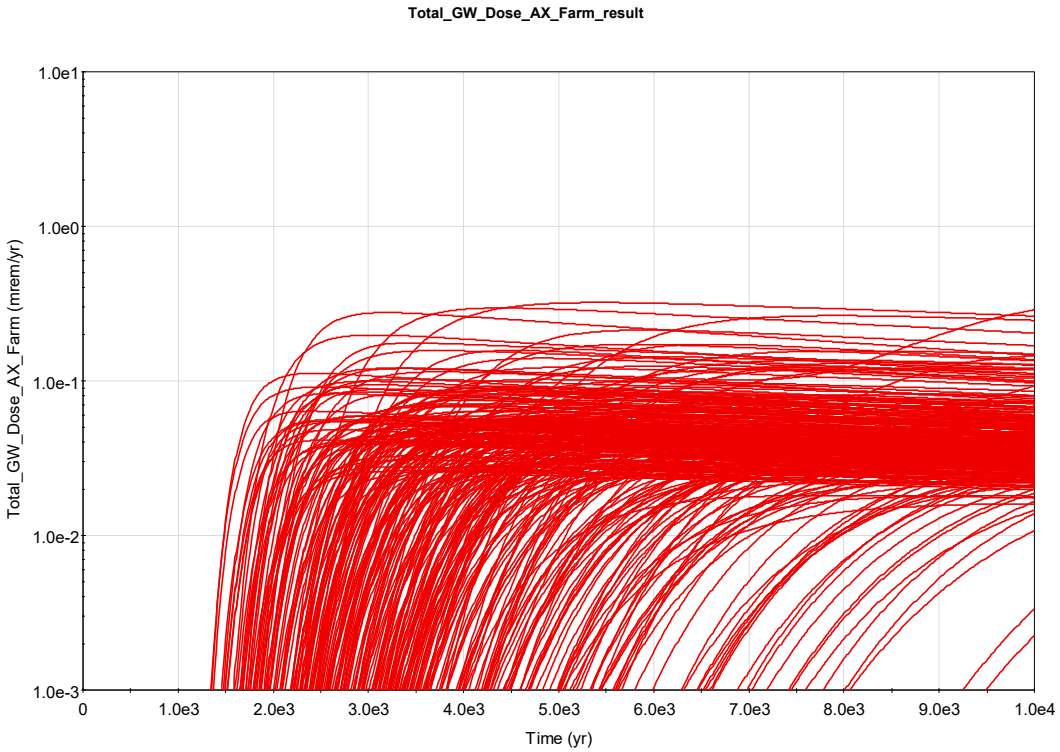
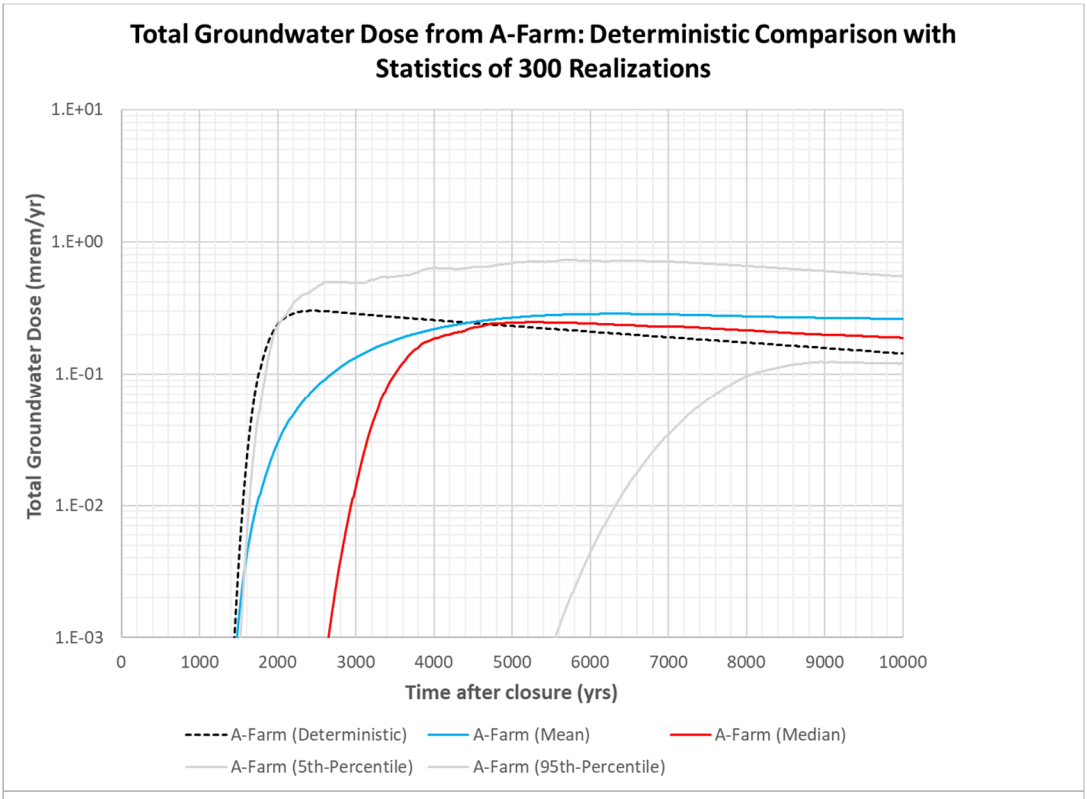


Figure 7-6. Comparison of Total Groundwater Dose Statistics for 300 Realizations: (a) 241-A Tank Farm, (b) 241-AX Tank Farm.

(a)



(b)

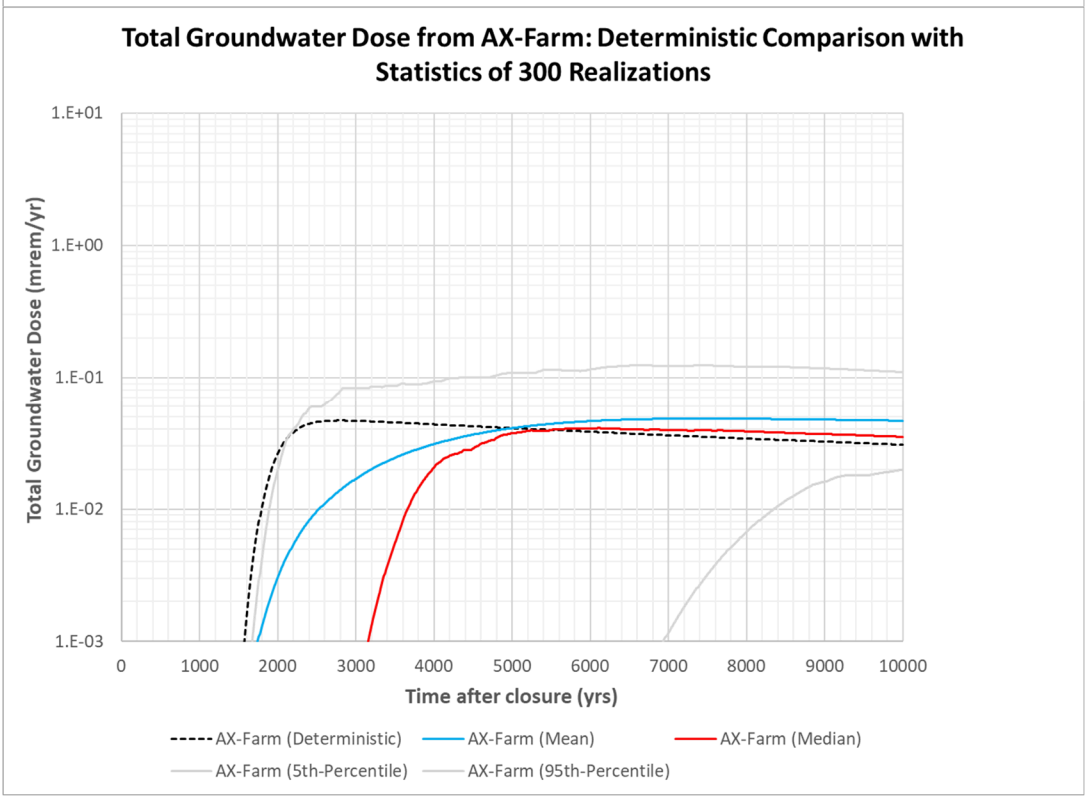


Figure 7-7. Total Groundwater Dose by Source: Comparison of Deterministic Model Run and Mean of 300 Realizations.

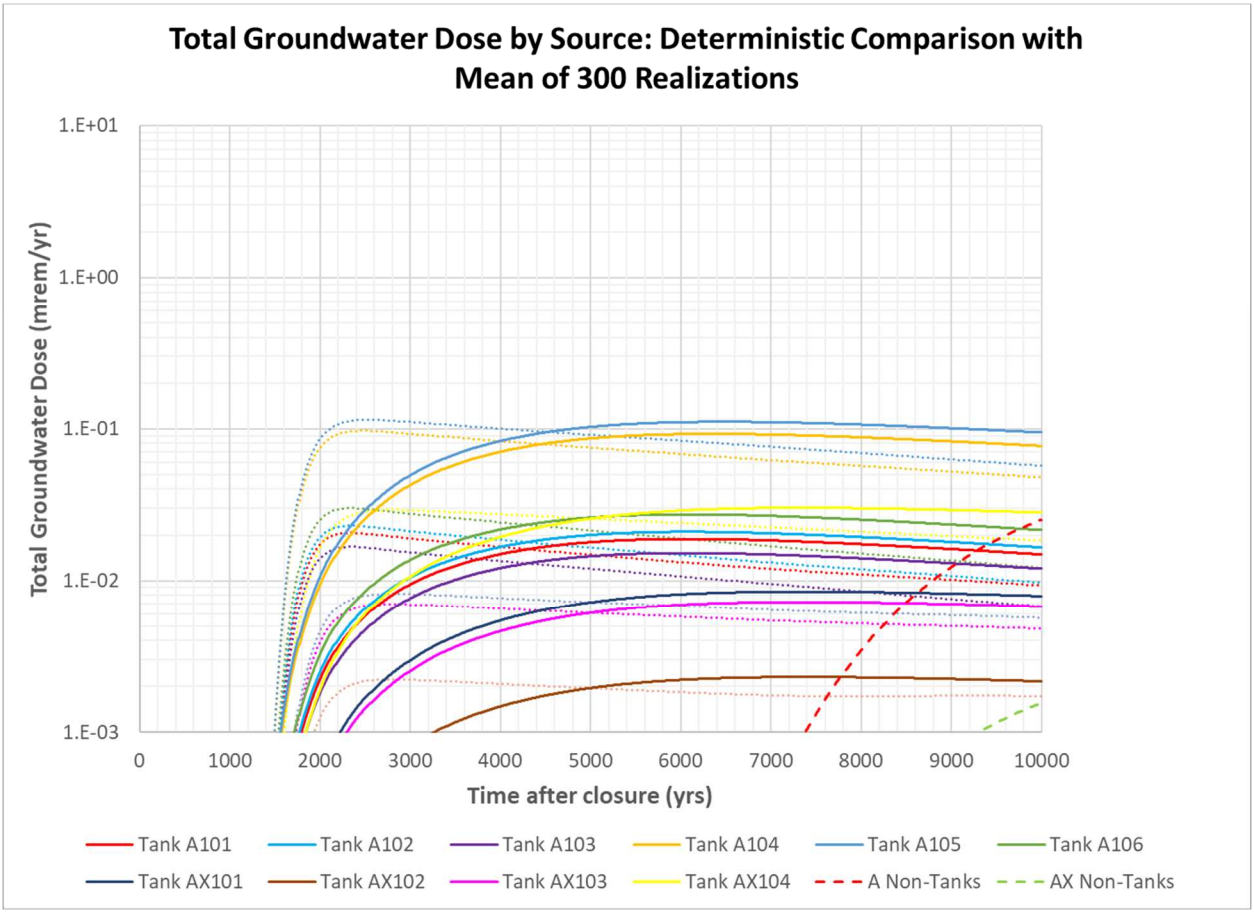


Figure 7-8. Total Groundwater Dose by Source: Comparison of Deterministic Model Run and Median of 300 Realizations.

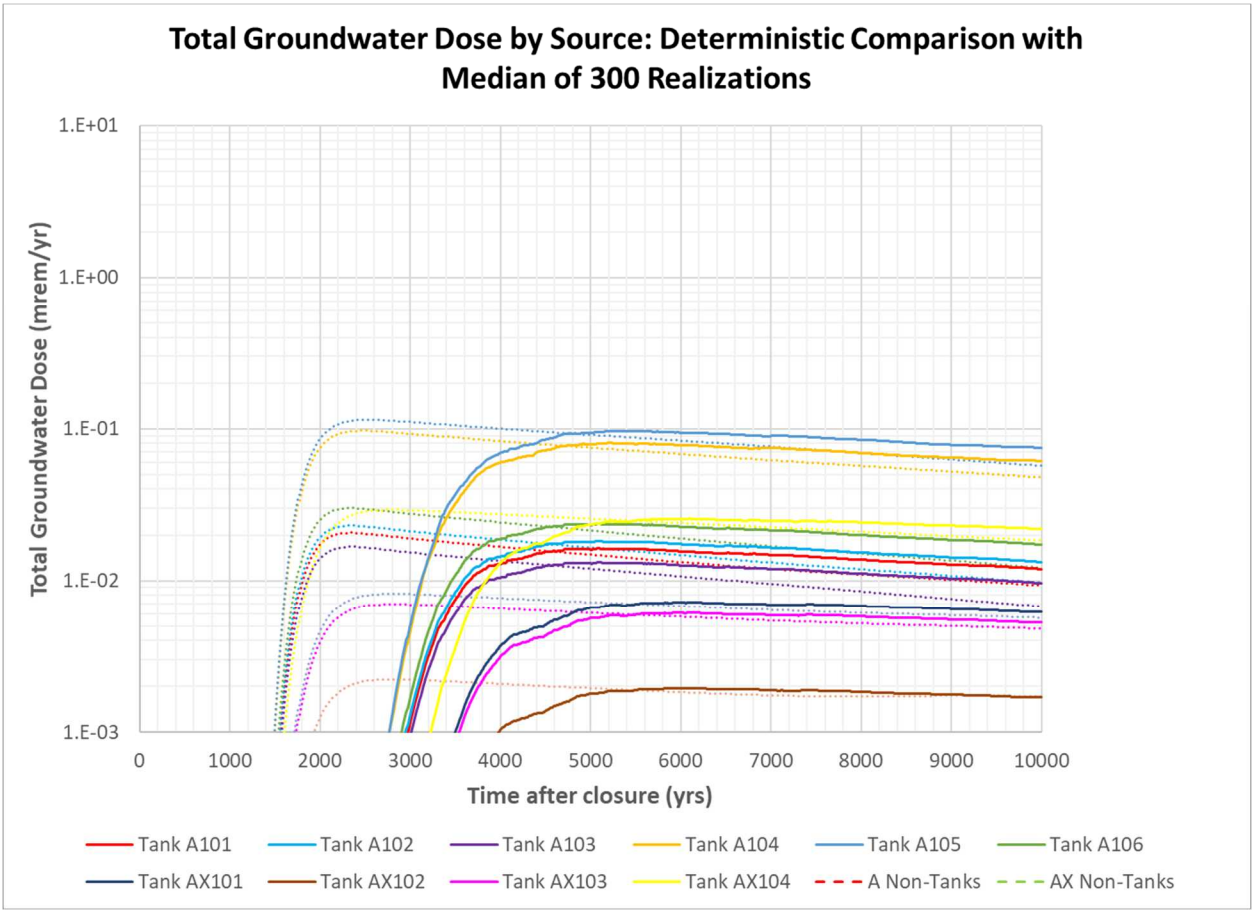


Figure 7-9. Total Groundwater Dose by Source: Comparison of Deterministic Model Run and 5th-Percentile of 300 Realizations.

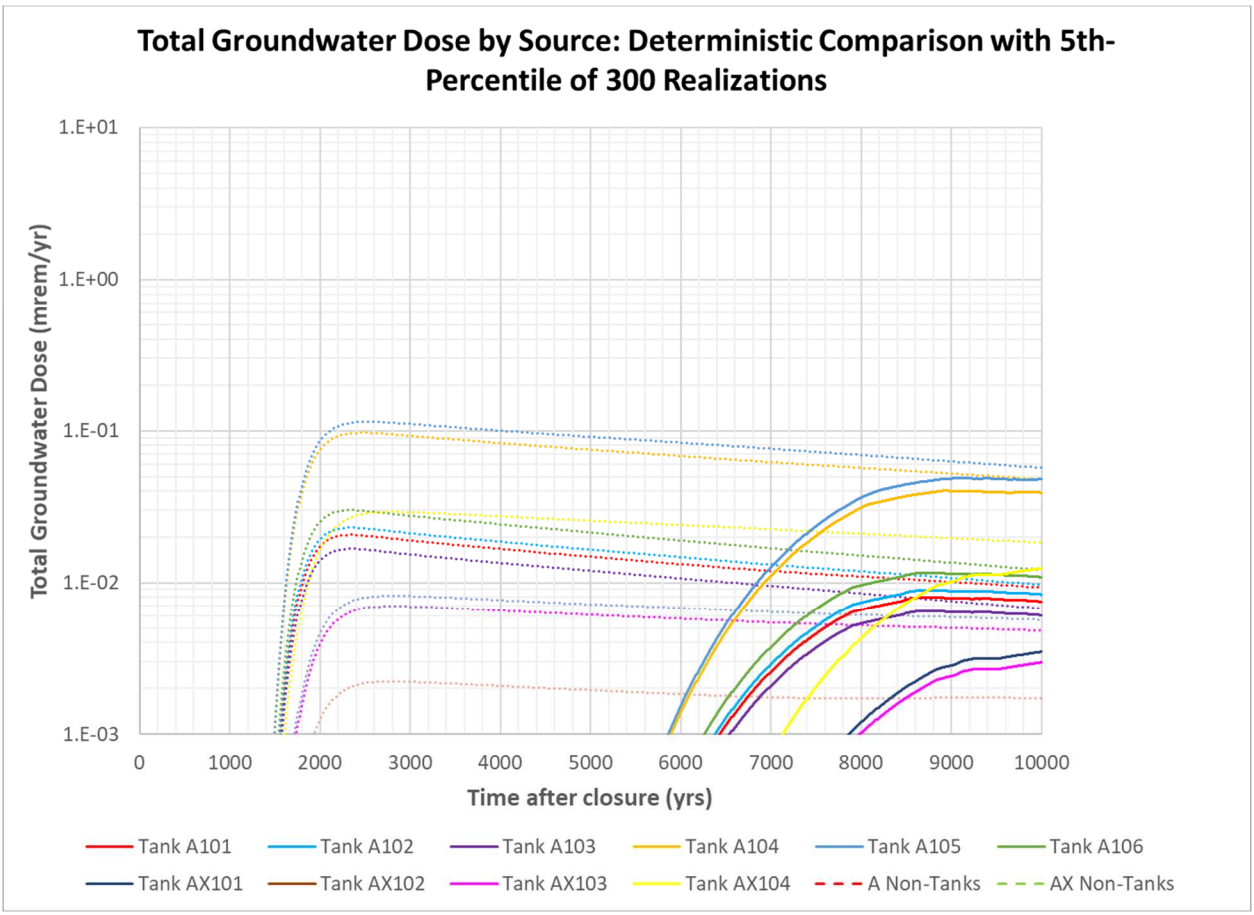
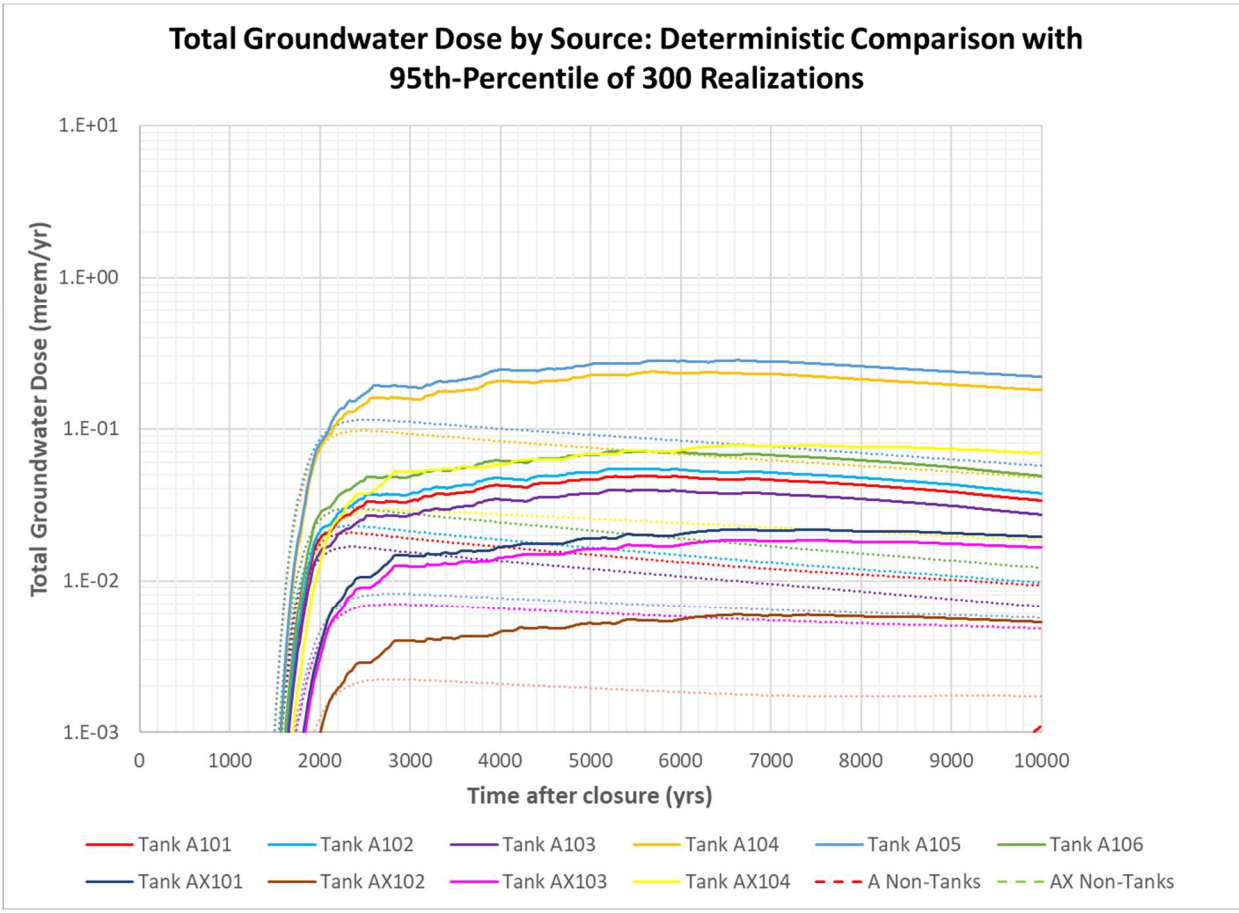


Figure 7-10. Total Groundwater Dose by Source: Comparison of Deterministic Model Run and 95th-Percentile of 300 Realizations.



7.3 RADIONUCLIDE GROUNDWATER DOSE ANALYSIS

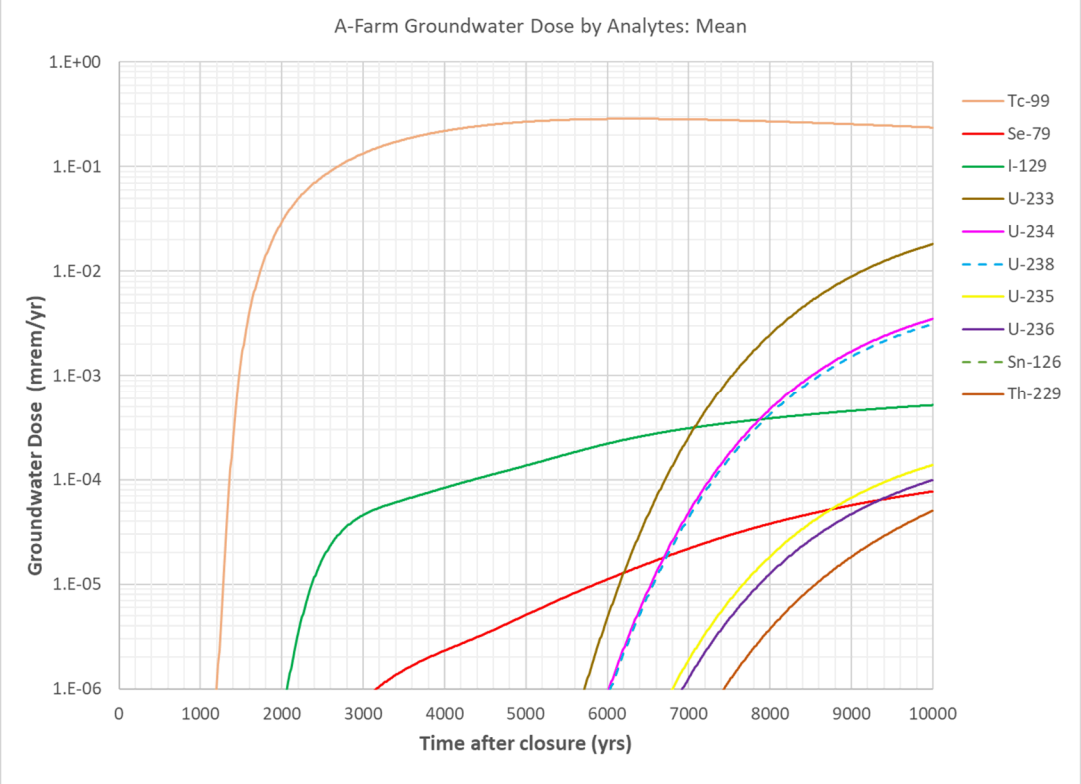
The total groundwater dose reported in Section 7.2 is the sum of the doses from the different radionuclides. There are 43 radionuclides included in the system model. Of these 43, 23 have no impact on groundwater in 10,000 years. These are: ^{241}Am, ^{243}Am, ^{113}Cd^{m}, ^{243}Cm, ^{244}Cm, ^{60}Co, ^{137}Cs, ^{152}Eu, ^{154}Eu, ^{155}Eu, ^{3}H, ^{59}Ni, ^{63}Ni, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{151}Sm, ^{90}Sr, ^{232}U, and ^{93}Zr. These radionuclides have no impact on the groundwater in 10,000 years either because there is no initial inventory of these radionuclides in the tank, their release and transport to the water table is significantly delayed by sorption, or their half-life is short and they decay before reaching the water table. For instance, americium, curium, plutonium, and zirconium all have minimum K_d values that are greater than or equal to 40 mL/g. These are radionuclides that do not impact the groundwater. However, thorium also has minimum K_d in this range but does impact the groundwater. Thorium impacts to the groundwater occur because thorium is transported as a more mobile species, for example uranium, which subsequently decays to thorium near to or after reaching the water table. Of the radionuclides that do reach the groundwater, the maximum doses from ^{14}C, ^{93}Nb^{m}, ^{228}Ra, and ^{232}Th are below 1×10^{-6} mrem/yr in any realization and will not be discussed.

This section identifies the key contributors to the total groundwater dose in the 300 realization run. The dose results discussed in this section are radionuclide doses from all sources in one of the two tank farms. Only ^{129}I, ^{226}Ra, ^{79}Se, ^{99}Tc, ^{229}Th, ^{233}U, ^{234}U, ^{235}U, ^{236}U, and ^{238}U have a peak dose result from at least one of the tank farms that exceeds 1×10^{-3} mrem/yr. Only ^{99}Tc, ^{233}U, ^{234}U, and ^{238}U have a peak dose result from at least one of the tank farms that exceeds 1×10^{-1} mrem/yr. These are the key contributors to the total groundwater dose.

In any Monte Carlo realization, ^{233}U has the highest groundwater dose (and is from the A-Tank Farm), followed by ^{99}Tc, ^{234}U, and then ^{238}U. Only ^{99}Tc has a peak groundwater dose from one of the tank farms that exceeds 0.1 mrem/yr in more than 5% of the realizations. In addition, ^{99}Tc is also the only radionuclide that exceeds 0.001 mrem/yr in more than 50% of the realizations. ^{129}I is the only other radionuclide that exceeds 0.001 mrem/yr in more than 5% of the realizations. Figure 7-11 shows the mean groundwater dose time histories for selected radionuclides from all sources in A Farm (a) and in AX Farm (b). Figure 7-12 shows the 95th-percentile groundwater dose time histories for selected radionuclides from all sources in A Farm (a) and in AX Farm (b). Plots for other percentiles only show ^{99}Tc above the 1×10^{-6} mrem/yr scale common to the figures. In lieu of presenting these results, scatter plots of the peak groundwater dose from each radionuclide are shown in Figure 7-13. These graphics show the distribution of peak radionuclide dose, but not the timing of the peak dose. For most radionuclides, the peak occurs near the end of the simulation. For ^{99}Tc, the peak occurs between 2,000 and 10,000 years after closure.

Figure 7-11. Mean Radionuclide Groundwater Dose for 300 Realizations: (a) 241-A Tank Farm, (b) 241-AX Tank Farm.

a



b

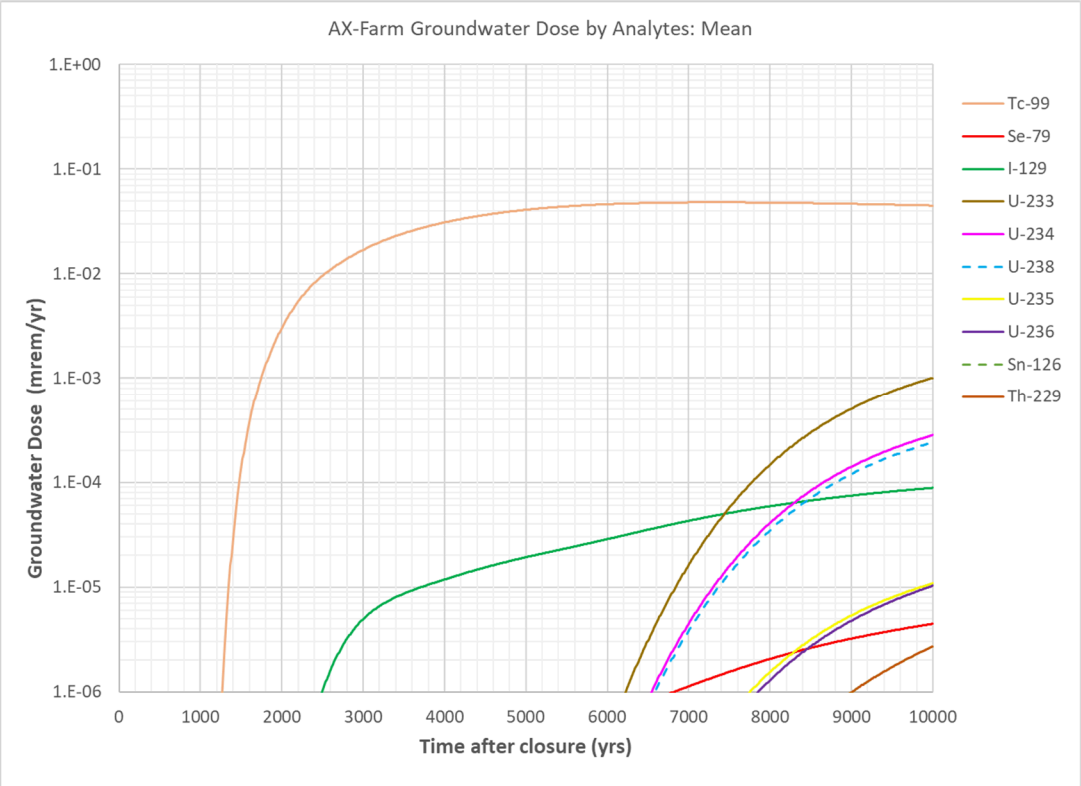
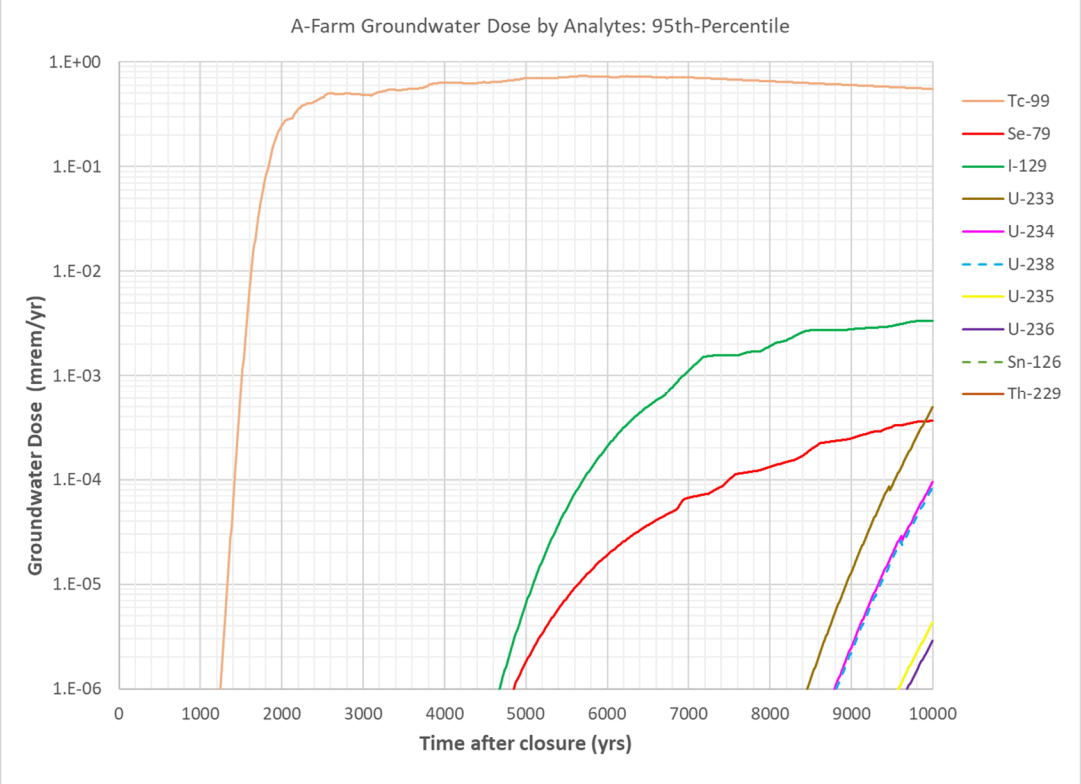


Figure 7-12. 95th-Percentile Radionuclide Groundwater Dose for 300 Realizations: (a) 241-A Tank Farm, (b) 241-AX Tank Farm.

a



b

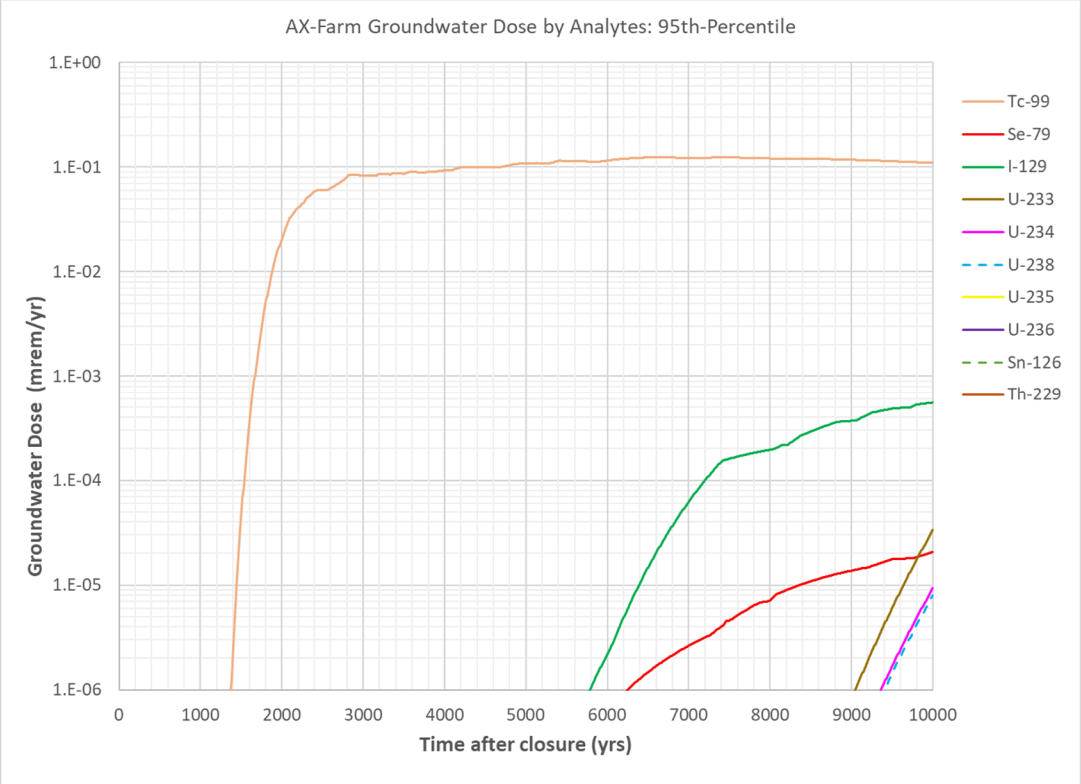
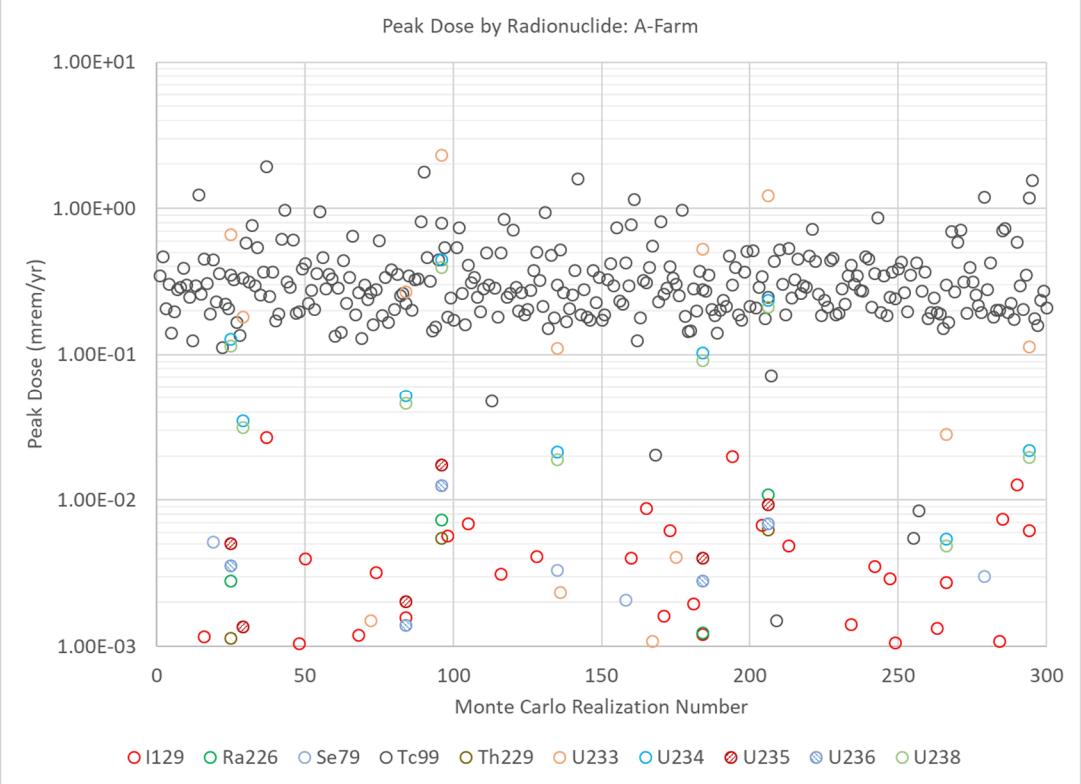
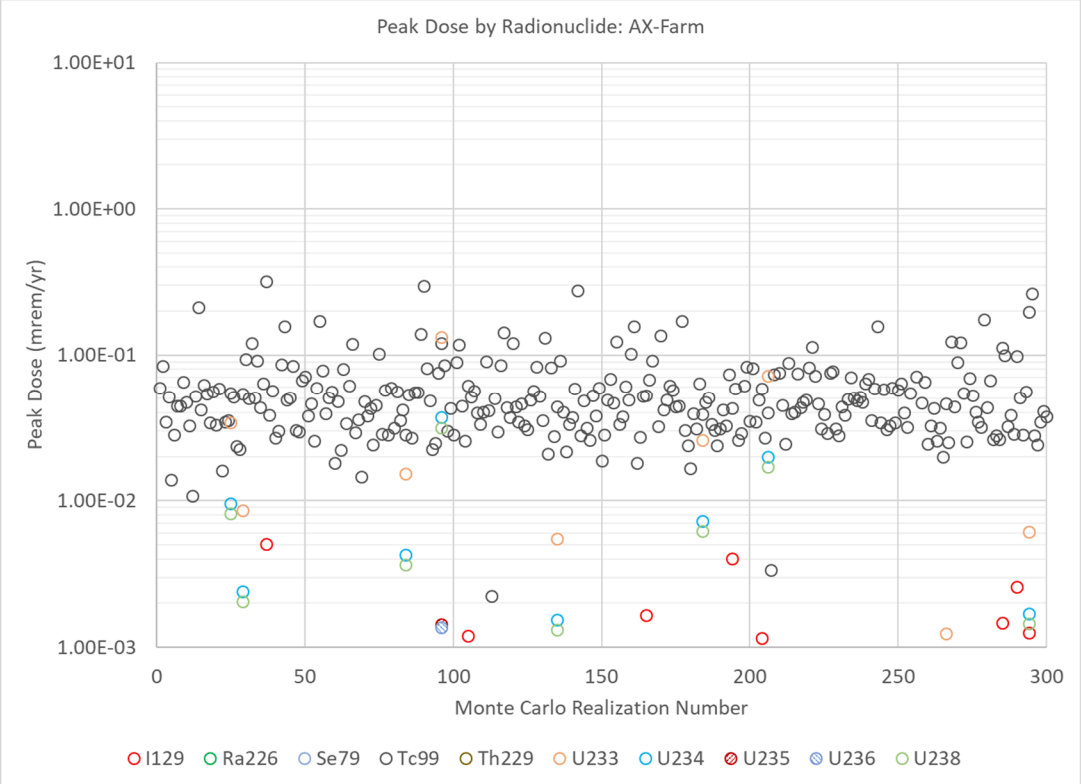


Figure 7-13. Distribution of Peak Radionuclide Groundwater Dose for 300 Realizations: (a) 241-A Tank Farm, (b) 241-AX Tank Farm.

a



b



7.4 CUMULATIVE RELEASE TO VADOSE ZONE ANALYSIS

The uncertainty in the groundwater dose from a radionuclide is governed by the uncertainty in the fate and transport processes pertaining to tank releases and migration through the natural system beneath the WMA. The uncertainty in tank release rates can be evaluated using the cumulative release from the tanks to the vadose zone. In this uncertainty analysis, the inventory is treated without uncertainty; therefore, the uncertainty in the total releases from tanks to the vadose zone is expected to be governed by diffusion coefficients and sorption coefficients for the waste. The uncertainty in the total releases from ancillary equipment to the vadose zone is expected to be governed by the net infiltration that flows through these components as well as the diffusion coefficients and sorption coefficients for the waste in these components.

Nitrate is used as a surrogate to understand the waste form release of a non-decaying, non-sorbing species. Cumulative releases of nitrate from tanks in A Farm are shown in Figure 7-14. The original inventory of nitrate in the A Farm tanks is 16,700 kg and after 10,000 years between 15,000 and 16,600 kg (90 to 99.4%) has been released to the vadose zone. Uncertainty in the diffusion coefficient through the grout is one of the causes of the range of results in the release histories. Releases from AX Farm tanks range from 99 to 100% of the initial inventory in the tanks. Releases from the non-tank sources in A Farm are shown in Figure 7-14b. Unlike releases from the tanks, which are assumed to be barriers to flow, the non-tank sources have advective releases. Therefore, 100% of the nitrate is released from the non-tank sources and it is released with very little uncertainty.
Releases of ^{99}Tc to the vadose zone from the tanks is controlled by uncertainty in the diffusion coefficient and uncertainty in the grout sorption coefficient. The grout sorption coefficient for ^{99}Tc ranges from 0.7 mL/g to 1.4 mL/g. Cumulative releases of ^{99}Tc from tanks in A Farm are shown in

Figure 7-15. The original inventory of ^{99}Tc in the A Farm tanks is 2.22 kg and after 10,000 years between 33 and 74% has been released to the vadose zone. Compared to 90 to 99% of nitrate being released, the lower fractions and wider range in the fraction of ^{99}Tc released is attributed to the sorption coefficient onto the grout. Releases from AX Farm tanks range from 19 to 59% of the initial inventory in the tanks. Similar to nitrate, 100% of the ^{99}Tc is released from the non-tank sources and it is released with very little uncertainty.

Similarly, release of ^{129}I from tanks is controlled by the same diffusion coefficient and its sorption coefficient onto the grout. The K_d for ^{129}I sorption onto grout ranges between 0.3 mL/g and 30 mL/g. The model results confirm that a lower fraction and wider range of ^{129}I is released from the A Farm tanks. With an initial inventory of 71 g, only between 3 and 69% is released to the vadose zone (see

Figure 7-16) from A Farm tanks and 1 to 46% is released from AX Farm tanks.
The uncertainty in the release of uranium from the tanks is governed by the uncertainty in the diffusion coefficient, the uncertainty in the sorption coefficient to grout, and the uncertainty in uranium solubility in the grout pore water. The initial inventory of ^{233}U in the A Farm tanks is 127 g, but less than 0.02% is released from the A Farm tanks in 10,000 years (see

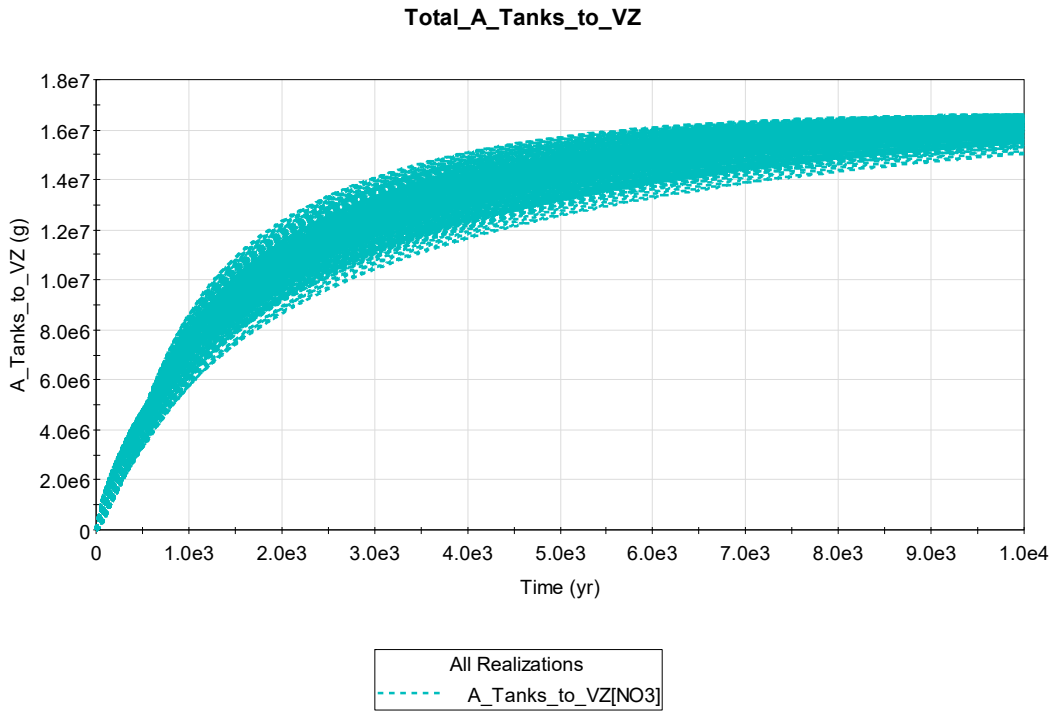
Figure 7-17). Fractions of a percent release also are observed from AX Farm tanks. Releases from the pipelines occur over a longer period, which is attributed to the imposed solubility limit. Unlike the other radionuclides referenced above, uranium releases from the non-tank sources are much greater than releases from the tanks. As illustrated in

Figure 7-17, there is very little uncertainty in the total amount of uranium released from these sources in 10,000 years. As a consequence, an importance analysis on the parameters that most significantly affect uranium release to the vadose zone in 10,000 years will not likely return any parameters because the releases to the vadose zone are dominated by a source that has very little uncertainty at the reference point. For this reason, an importance analysis performed on total uranium release to the vadose zone should isolate tank and non-tank sources and/or perform the evaluation for an intermediate time point, such as the DOE time of compliance at 1,000 years.

Figure 7-18 shows the fraction of the initial inventory that is released to the vadose zone from all sources in the WMA before it decays. Radionuclides with fractions that exceed one are decay products that are generated in the source prior to being released to the vadose zone. The marker shows the minimum and maximum in the range of results for the 300 realization case together with the mean. Radionuclides with a range that does not extend much above and below the mean have very little uncertainty in total release to the vadose zone.

Figure 7-14. Cumulative Release to the Vadose Zone from 241-A Farm Tanks (a) and Non-Tanks (b): 300 Realizations, Nitrate.

a



b

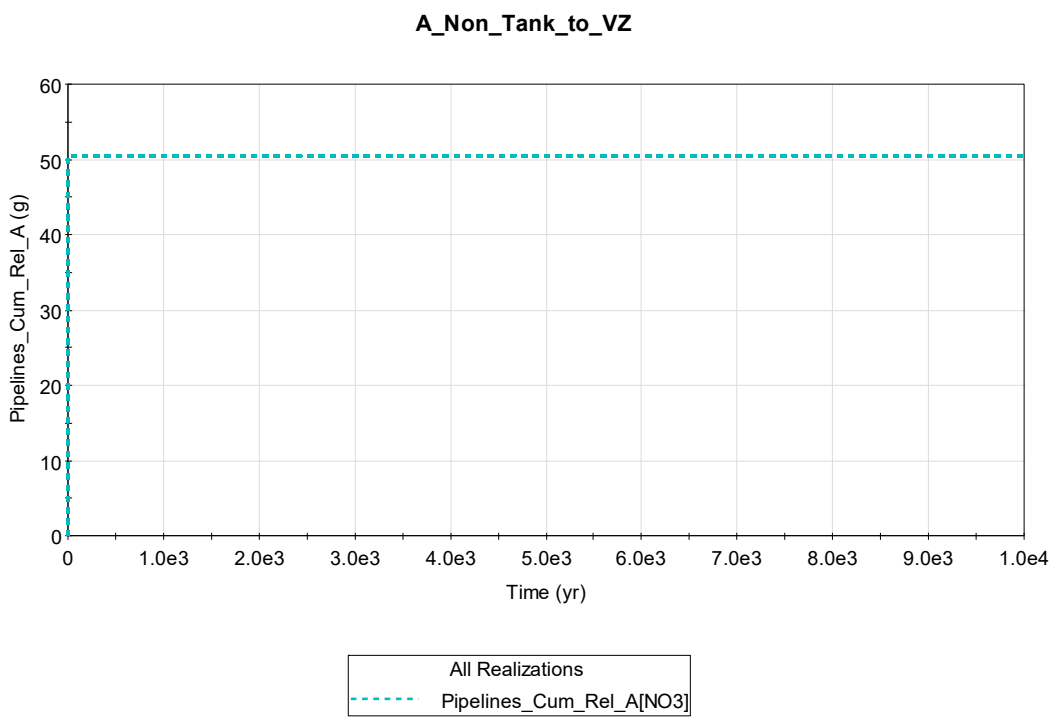
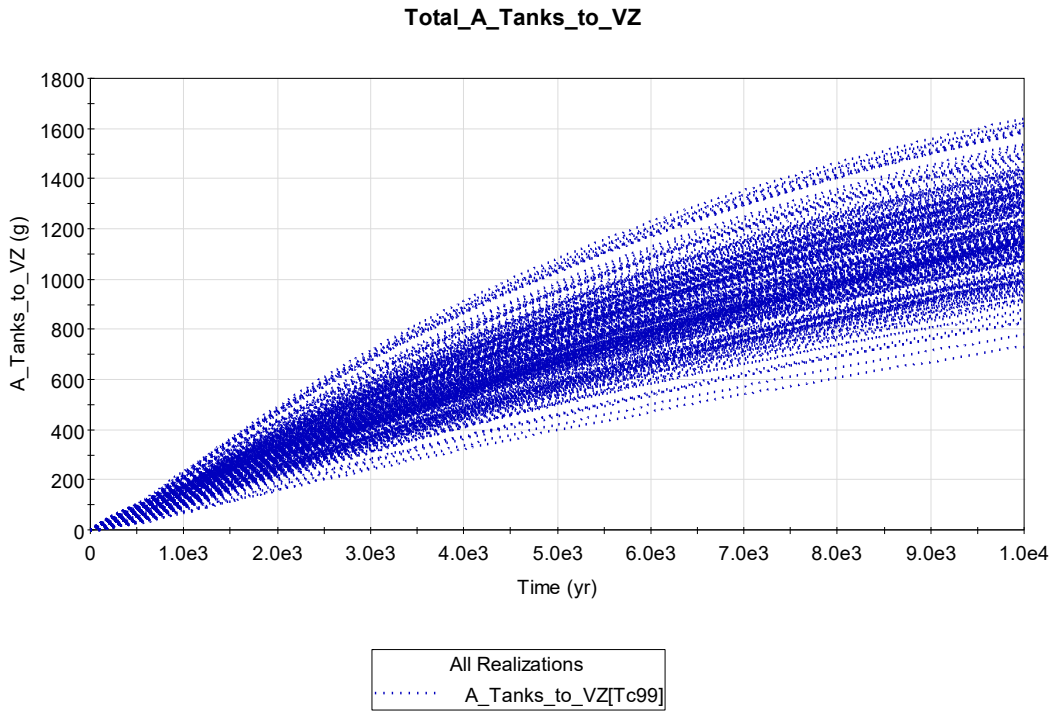


Figure 7-15. Cumulative Release to the Vadose Zone from 241-A Farm Tanks (a) and Non-Tanks (b): 300 Realizations, Technetium-99.

a



b

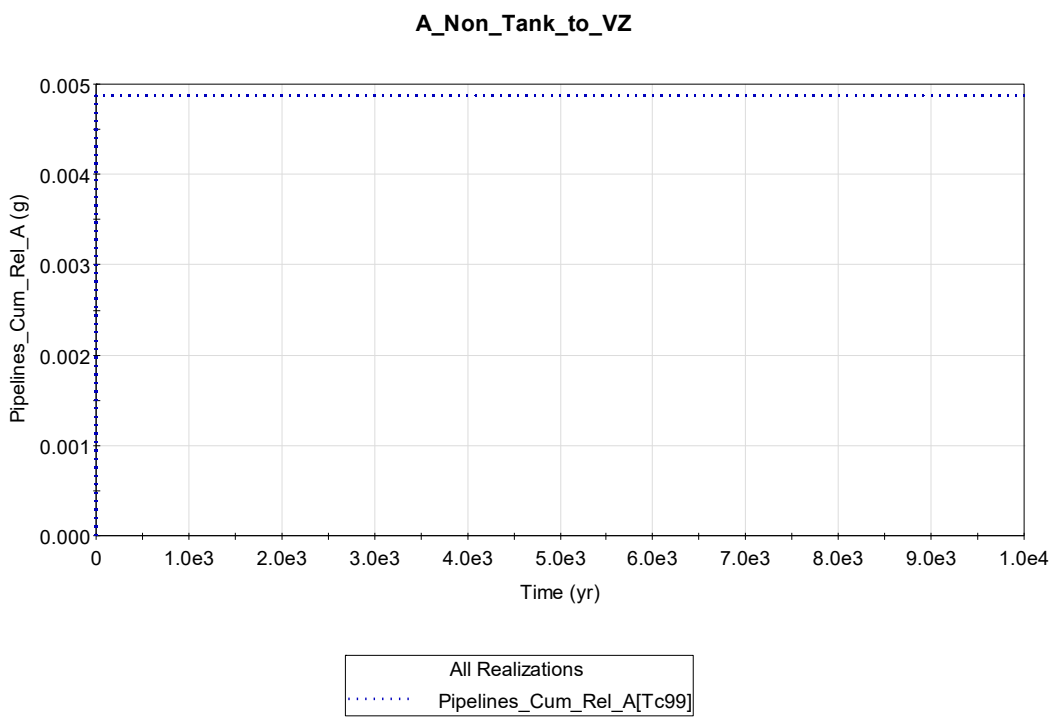
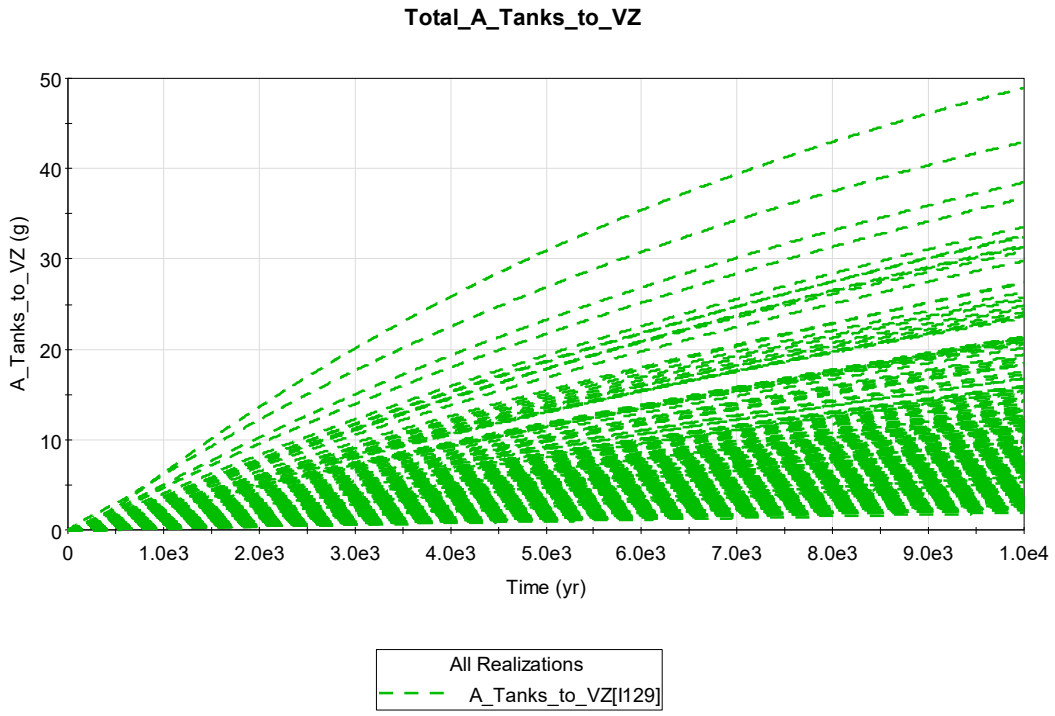


Figure 7-16. Cumulative Release to the Vadose Zone from 241-A Farm Tanks (a) and Non-Tanks (b): 300 Realizations, Iodine-129.

a



b

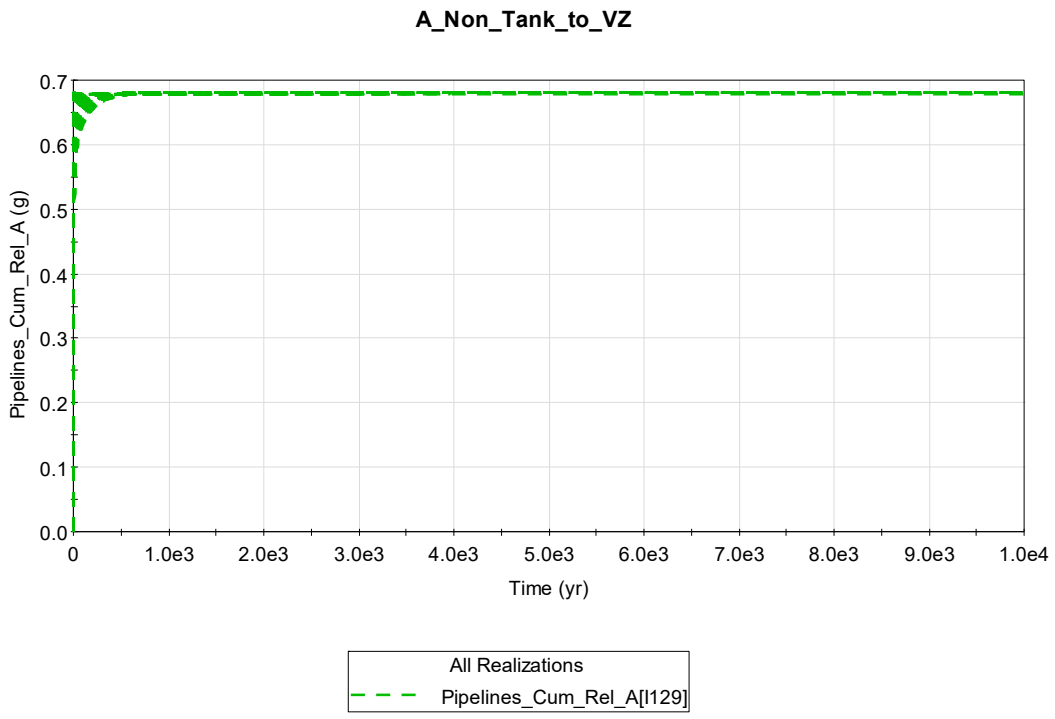
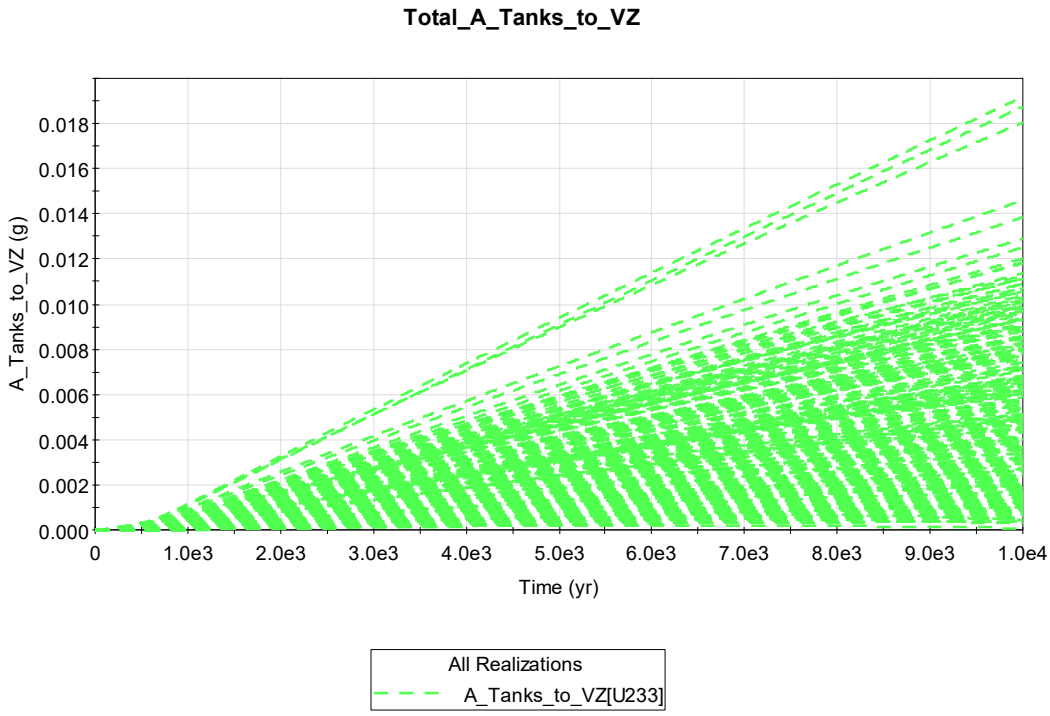


Figure 7-17. Cumulative Release to the Vadose Zone from 241-A Farm Tanks (a) and Non-Tanks (b): 300 Realizations, Uranium-233.

a



b

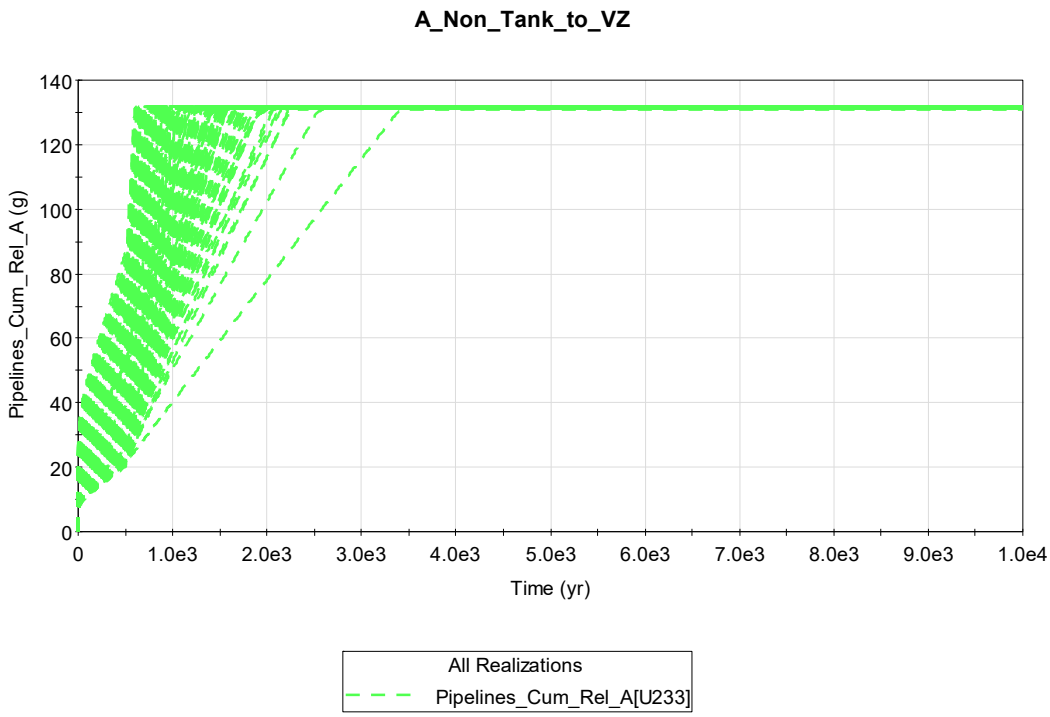
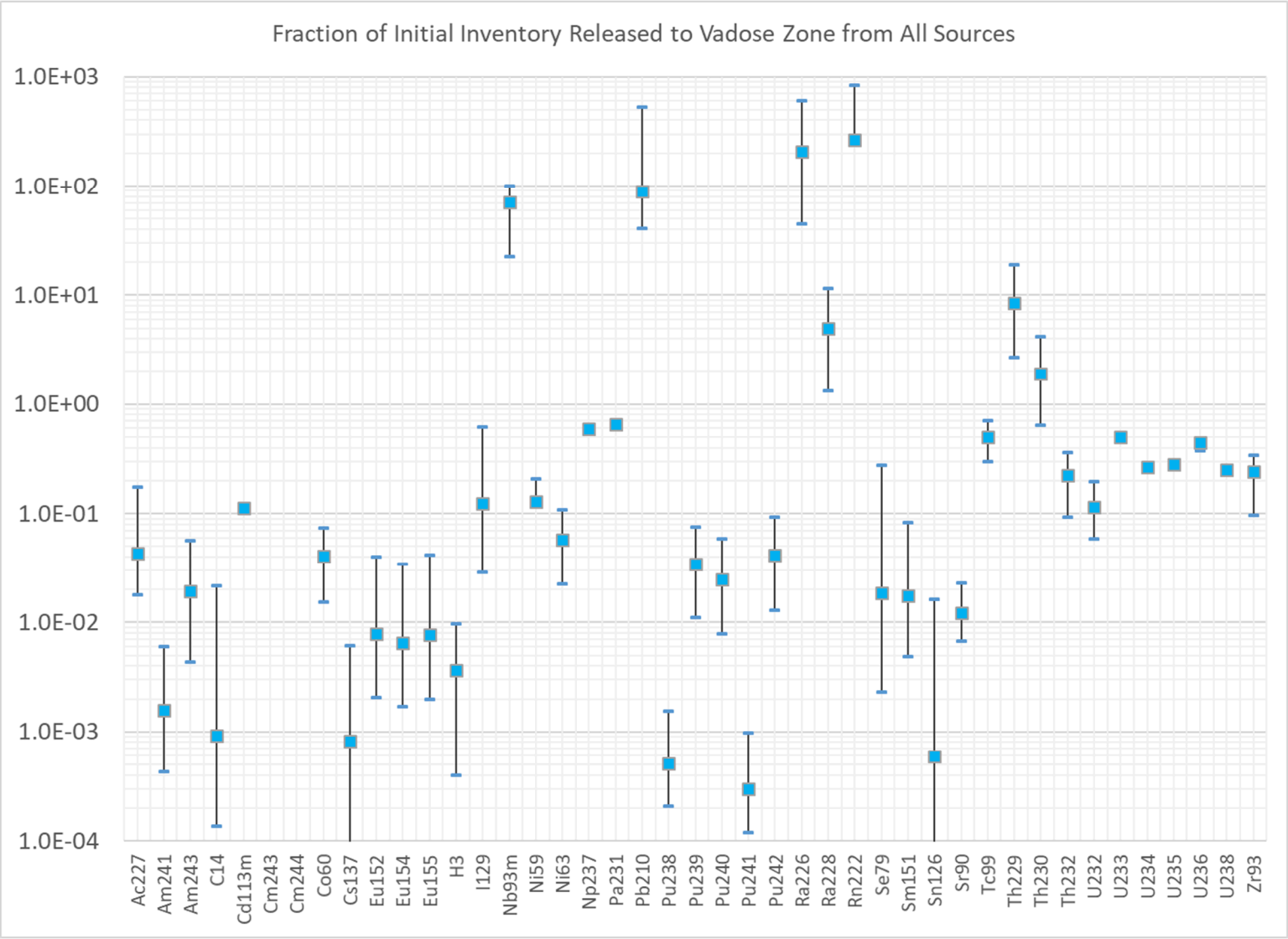


Figure 7-18. Uncertainty in the Cumulative Release to the Vadose Zone from All Sources: Minimum, Mean, and Maximum.



7.5 CUMULATIVE RELEASE TO SATURATED ZONE ANALYSIS

Once a constituent is released from the tank or non-tank sources, it must travel through the partially-saturated vadose zone. Sorption to the sediments under the WMA may prolong transport times such that all the mass that is released to the vadose zone may not reach the water table in 10,000 years. Uncertainty in the travel times will be governed by the uncertainty in the net infiltration rate that changes the flow fields underneath the WMA, as well as uncertainty in the sorption coefficients.

Figure 7-19 shows the cumulative release histories for nitrate, which travels through the vadose zone without retardation due to sorption. Uncertainty in the cumulative amount of nitrate released from the vadose zone to the saturated zone will be governed by the flow fields underneath the WMA. Compared to the cumulative amount of nitrate released to the vadose zone (90 to 99%), the cumulative release to the saturated zone is reduced. The cumulative release of nitrate to the saturated zone from the A Farm tanks ranges from 0.1 to 99% of the initial inventory. The cumulative release of nitrate to the saturated zone from the non-tank sources in A Farm range from 1.1 to 100% of the initial inventory.

Similar to nitrate, when compared to releases from the sources, releases of ^{99}Tc, ^{129}I, and ^{233}U to the saturated zone are all delayed in time and lower in value. Figure 7-20 shows the cumulative release to the water table for ^{99}Tc, Figure 7-21shows ^{129}I, and Figure 7-22 shows ^{233}U.

Transport of ^{99}Tc to the water table through the deep vadose zone is governed by the vadose zone flow field, which is correlated to the net infiltration rate, and the sorption coefficient to the subsurface sediments. Before applying a gravel correction to reduce the effective K_d through the Hanford lithological units, the K_d for ^{99}Tc ranges from 0 to 0.1 mL/g. Gravel-corrected values reduce the maximum K_d value from 0.1 mL/g to 0.09 mL/g in Hanford sands (Hanford formation units 1 and 2 [H1 and H2]) and 0.032 mL/g in Hanford gravels (Hanford formation unit 3 [H3] and Cold Creek unit gravel [CCUg]). Gravel-corrected values for silt (Cold Creek unit silt [CCUz]) range from 0 to 0.097 mL/g. The cumulative release of ^{99}Tc to the saturated zone from the A Farm tanks ranges from ~0 to 67% of the initial inventory. The cumulative release of ^{99}Tc to the saturated zone from the non-tank sources in A Farm ranges from 0.5 to ~100% of the initial inventory.

Transport of ^{129}I to the water table through the deep vadose zone is governed by the vadose zone flow field and the sorption coefficient to the subsurface sediments. Before applying a gravel correction to reduce the effective K_d through the Hanford lithological units, the K_d for ^{129}I ranges from 0 to 2 mL/g. Gravel-corrected values reduce the maximum K_d value from 2 m L/g to 1.85 mL/g in Hanford sands (H1 and H2) and 0.66 mL/g in Hanford gravels (H3 and CCUg). Gravel-corrected values for silt (CCUz) range from 0 to 1.94 mL/g. The cumulative release of ^{129}I to the saturated zone from the A Farm tanks ranges from 0 to 40% of the initial inventory. The cumulative release of ^{129}I to the saturated zone from the non-tank sources in A Farm ranges from 0 to ~99% of the initial inventory.

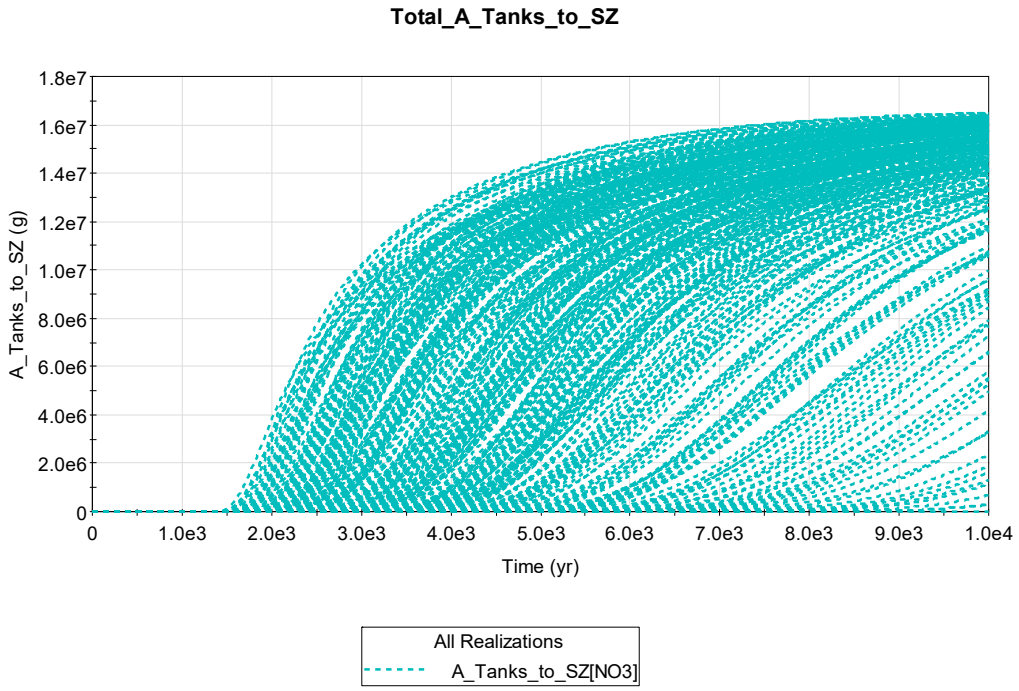
Transport of ^{233}U to the water table through the deep vadose zone is governed by the vadose zone flow field and the sorption coefficient to the subsurface sediments. Solubility limits are

imposed on uranium transport in the natural system, but the limits are higher than in the waste form so uranium transport is not affected by solubility limits in the vadose zone. Before applying a gravel correction to reduce the effective K_d through the Hanford lithological units, the K_d for ^{233}U ranges from 0.2 to 2 mL/g. Gravel-corrected values reduce the maximum K_d value from 2 mL/g to 1.87 mL/g in Hanford sands (H1 and H2) and 0.67 mL/g in Hanford gravels (H3 and CCUg). Gravel-corrected values for silt (CCUz) range from 0.2 to 1.92 mL/g. The cumulative release of ^{233}U to the saturated zone from the A Farm tanks ranges from 0 to 0.00025% of the initial inventory. The cumulative release of ^{233}U to the saturated zone from the non-tank sources in A Farm range from 0 to 40% of the initial inventory. The initial inventory value used in the comparison is not adjusted for ^{233}U that is produced as a decay product of ^{237}Np, ^{241}Am, and ^{241}Pu.

Figure 7-23 shows the fraction of the initial inventory that is released to the saturated zone from all sources in the WMA before it decays. Radionuclides with fractions that exceed one are decay products that are generated in the source or vadose zone prior to being released to the saturated zone. The marker shows the minimum and maximum in the range of results for the 300 realization case together with the mean. Radionuclides with a range that does not extend much above and below the mean have very little uncertainty in total release to the saturated zone. Radionuclides without a minimum value have a zero minimum value that does not show up on a logarithmic axis. The cumulative release of a specific radionuclide does not account for radionuclide decay once the radionuclide has been transported past the point of evaluation.

Figure 7-19. Cumulative Release to the Saturated Zone from 241-A Farm Tanks (a) and Non-Tanks (b): 300 Realizations, Nitrate.

(a)



(b)

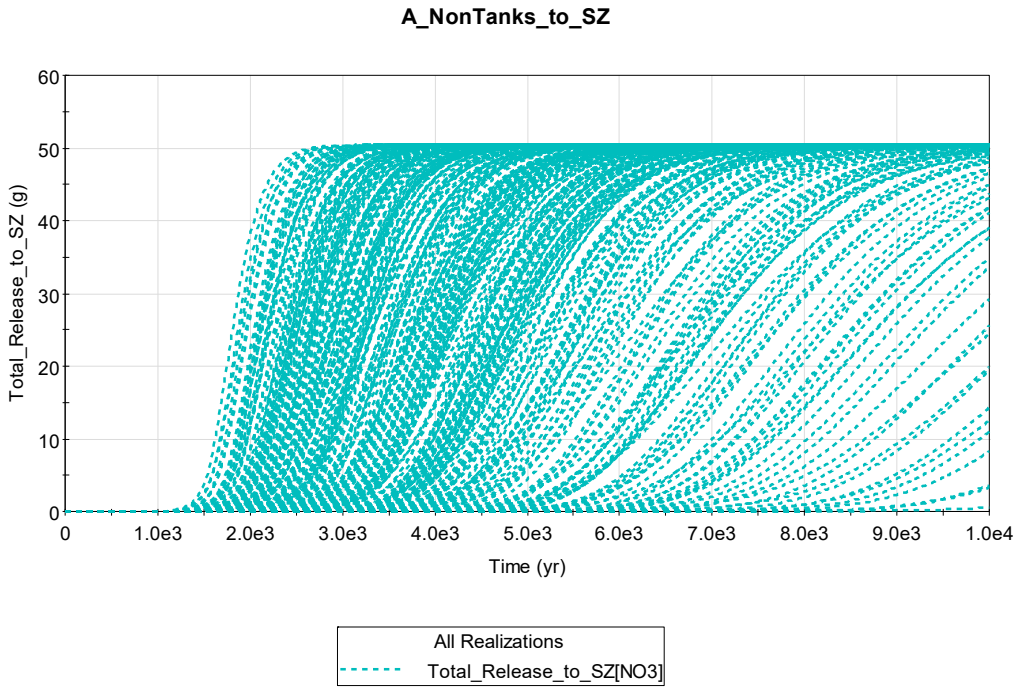
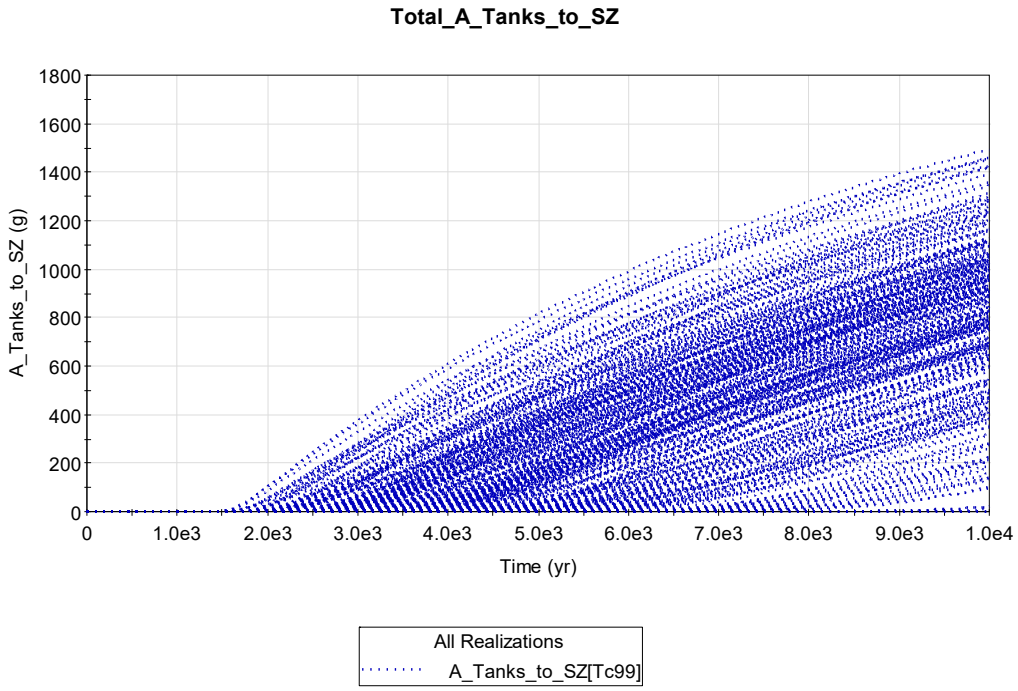


Figure 7-20. Cumulative Release to the Saturated Zone from 241-A Farm Tanks (a) and Non-Tanks (b): 300 Realizations, Technetium-99.

(a)



(b)

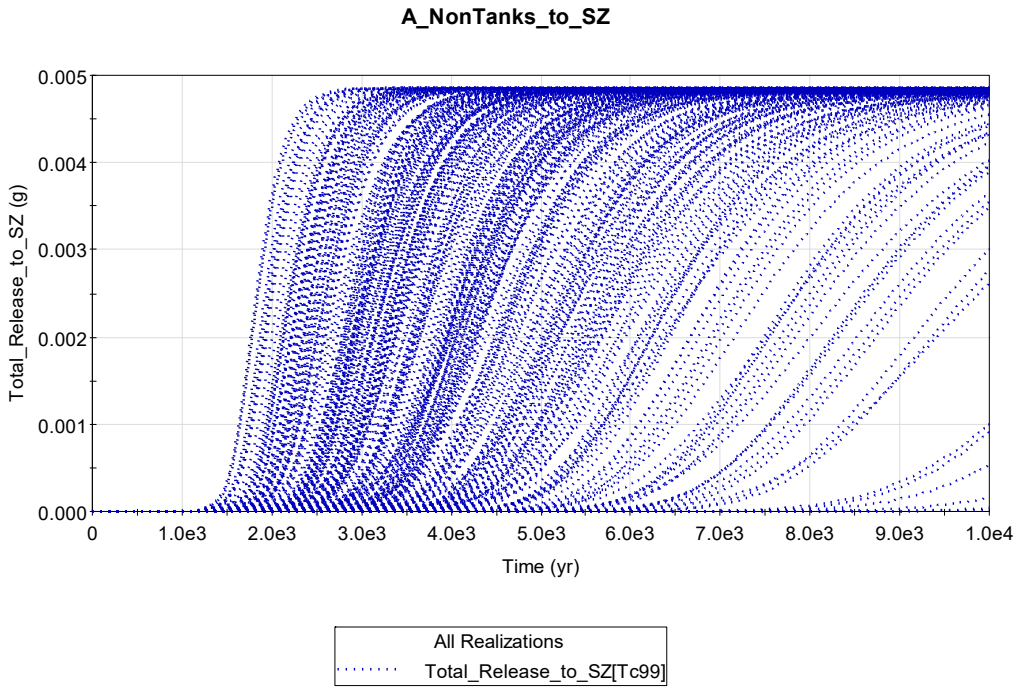
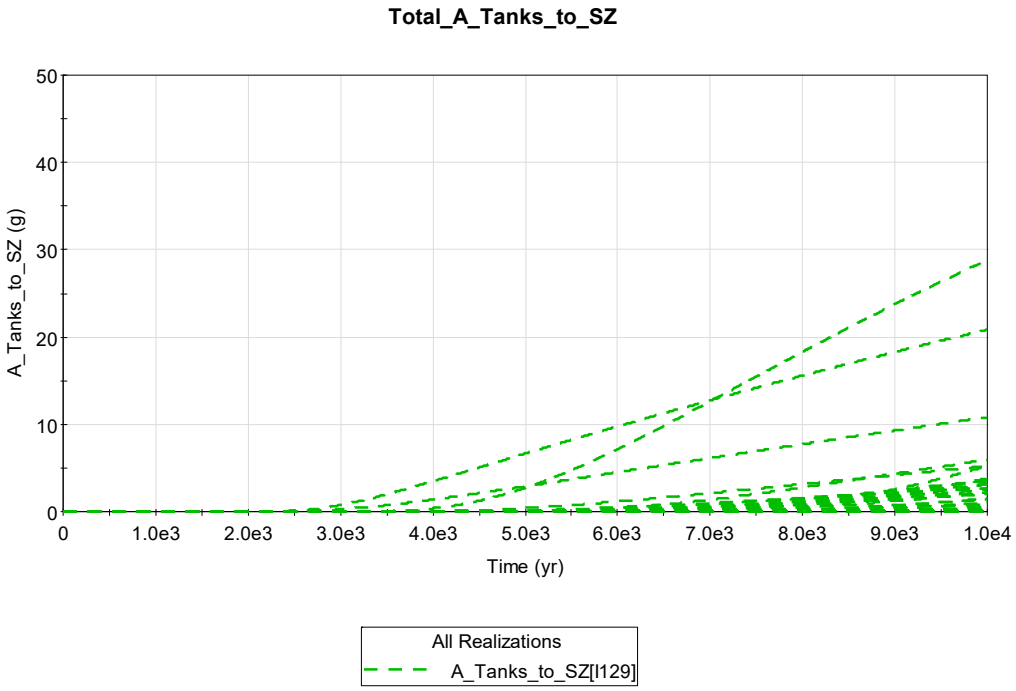


Figure 7-21. Cumulative Release to the Saturated Zone from 241-A Farm Tanks (a) and Non-Tanks (b): 300 Realizations, Iodine-129.

(a)



(b)

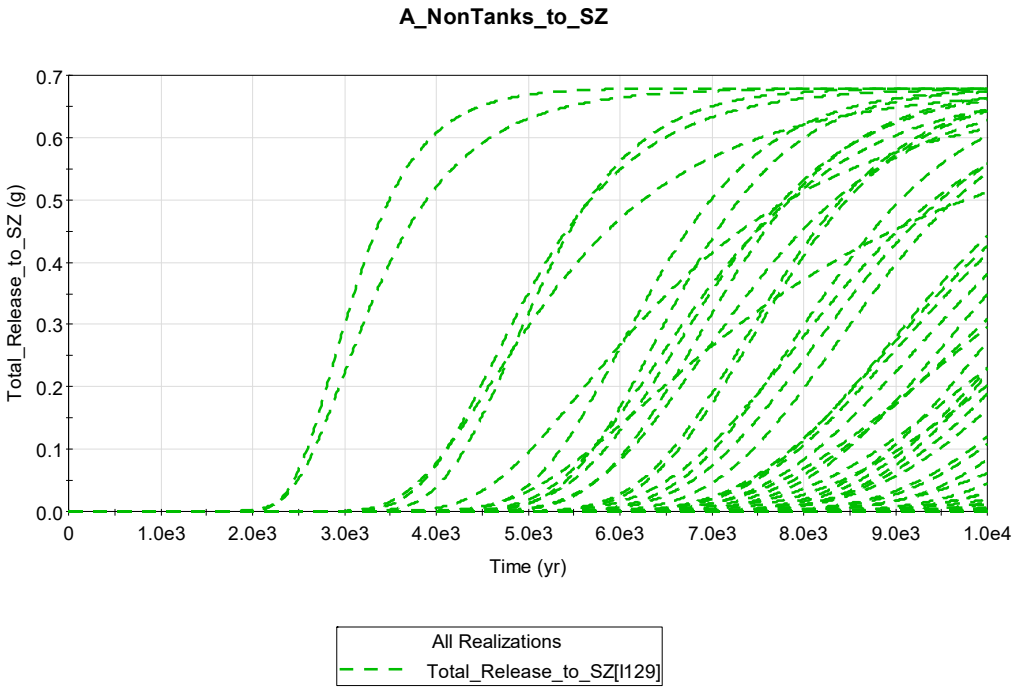
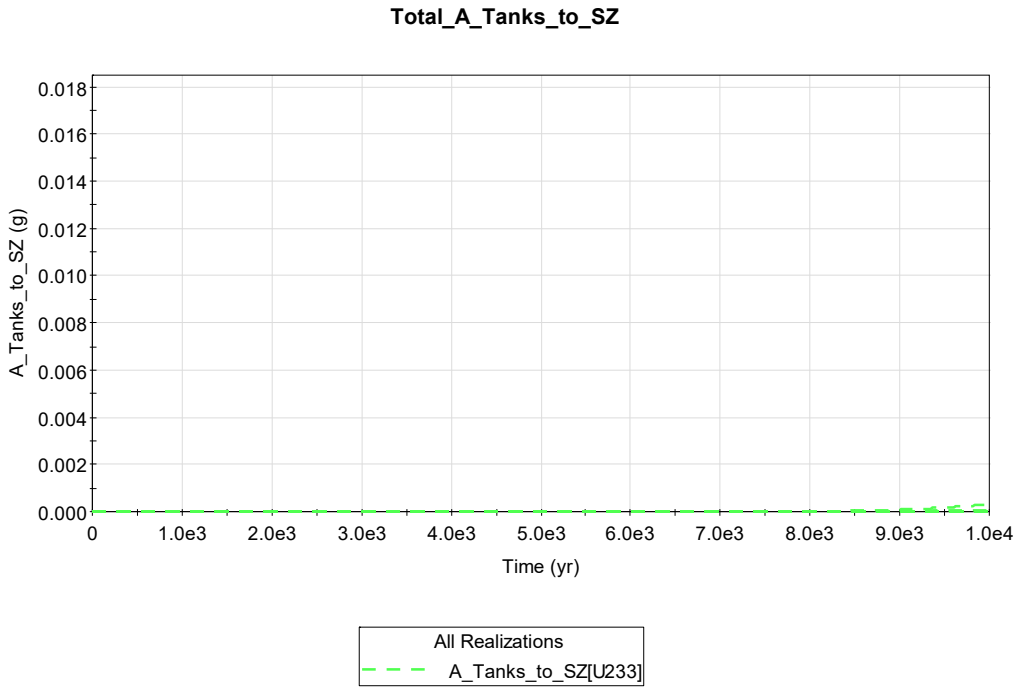


Figure 7-22. Cumulative Release to the Saturated Zone from 241-A Farm Tanks (a) and Non-Tanks (b): 300 Realizations, Uranium-233.

(a)



(b)

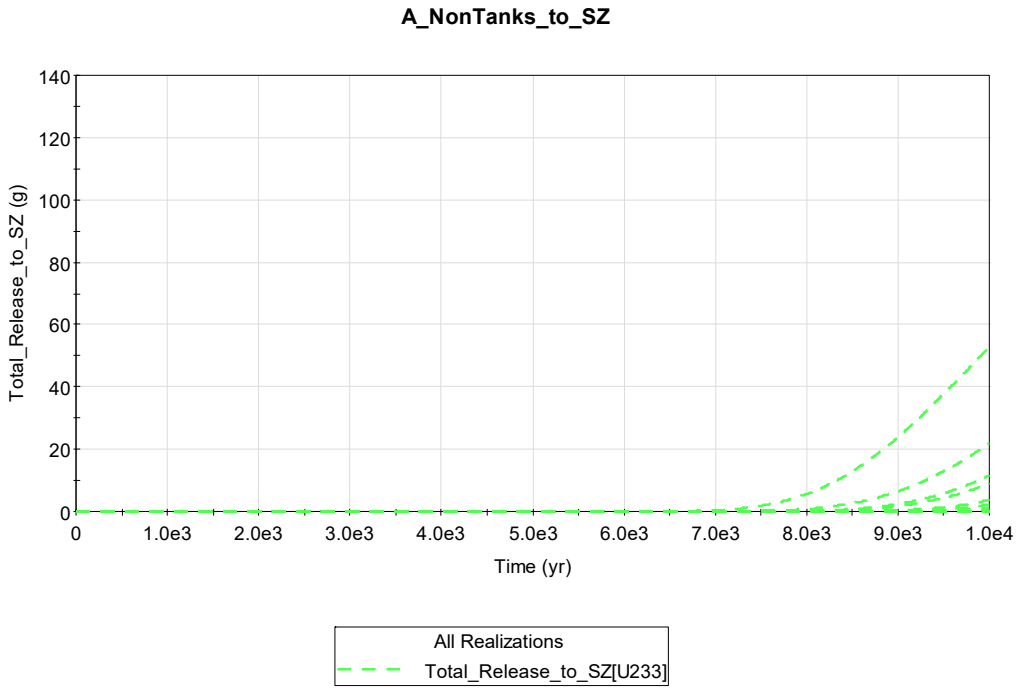
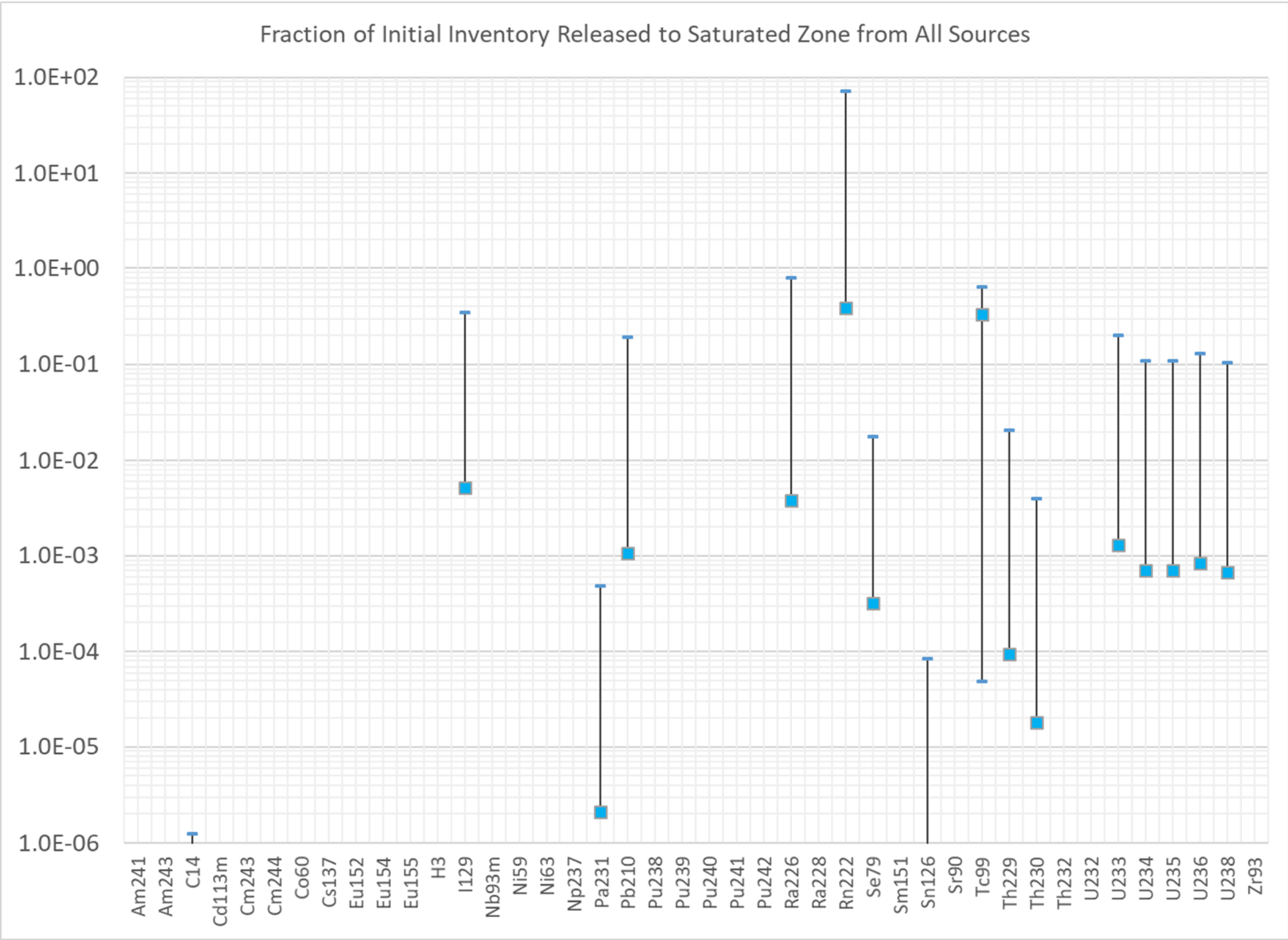


Figure 7-23. Uncertainty in the Cumulative Release to the Saturated Zone from All Sources: Minimum, Mean, and Maximum.



NOTE: For radionuclides with no minimum value depicted, the minimum cumulative release fraction was 0, which does not render on a logarithmic scale. Radionuclides with he a maximum value greater than unity, are decay products whose inventory can increase because of radionuclide decay.

7.6 IMPORTANCE ANALYSIS

NCRP Report 152 defined importance analysis as

> *"Importance analysis is an integration and interpretation of results obtained from the performance assessment process for the purpose of identifying assumptions and parameters which, when changed within credible bounds, can affect a decision about regulatory compliance." (NCRP Report 152 page 6)*

An importance analysis evaluates the strength of the correlation between an uncertain parameter and the uncertainty in a specified outcome. Many different statistical techniques can be applied to evaluate the strength of the correlations. In this analysis the correlation capabilities in the GoldSim© software provide the primary tool for evaluating key parameter uncertainties with corroboration by other methods. Two other methods are applied: (1) stepwise regression and (2) "random forest" analysis.

7.6.1 GoldSim© Sensitivity Metrics

The GoldSim© software provides statistical sensitivity analysis capabilities through a multivariate result display element. The element computes a coefficient of determination between an output and an input, a correlation coefficient, a standardized regression coefficient, a partial correlation coefficient, and an Importance Measure. Computational details of each sensitivity measure are described in Appendix B of the GoldSim© User Manual.

Coefficient of Determination represents the fraction of the total variance in a result that can be explained assuming a linear relationship between the input variables and the output result ($R = C_1X_1+C_2X_2+C_3X_3+ \ldots$). The closer the value is to unity, the better that a linear combination of the input parameters can be used to predict the output result.

Correlation coefficients quantify the degree of linearity between an input and an output result. Correlation coefficients range between -1 and 1; values near 1 and -1 represent a strong linear response between the input and the output. Positive values reveal a positive correlation between the input and output; as the input increases, the output increases. Conversely, negative values reveal a negative correlation; as the input increases, the output decreases. Correlation coefficients near zero signify little or no correlation between the input and the output. Correlation coefficients can be based on the actual raw values of the parameters and result or a rank of the parameters and result. In the rank correlation approach, the lowest value of a given input or output is given the rank 1 and sequential ranks are assigned based on the input or output values in ascending order. The rank of the highest value is equal to the number of Monte Carlo realizations that were performed.

Standardized Regression Coefficients are correlation coefficients determined after transforming the raw values of the input and output. The transformation normalizes the raw values by subtracting the sample mean from the raw value and then divides the difference by the sample standard deviation.

Partial correlation coefficients reflect the extent to which there is a linear relationship between the selected result and an input variable, after removing the effects of any linear relationships between the other input variables and both the result and the input variable in question.

If there is a nonlinear, non-monotonic relationship between an input variable and the result, conventional correlation coefficients may not reveal the relationship. The Importance Measure computed by GoldSim© is a normalized measure of the expected value of the variance if the input variable was not uncertain. The measure represents the fraction of the result variance that is explained by each input variable and can be calculated using raw values or ranks. The higher the value of the Importance Measure, the stronger correlation between the input and the output.

A multivariate element was added to the model that has a target output as the peak total dose from A Farm sources and all 117 uncertain inputs.

7.6.1.1 Summary of Results for Total Groundwater Dose from 241-A Tank Farm Sources

An importance analysis using the sampled values from all of the uncertain parameters was performed for the peak total groundwater dose from all A Farm sources. Table 7-2 provides a summary of the different methods for assessing the importance of the different uncertainty parameters. All four methods reveal a strong correlation between the saturated zone Darcy flux and the recharge rate under a degraded surface barrier.

Table 7-2. Peak Total Groundwater Dose from 241-A Tank Farm Sources: Importance Analysis Results.

GoldSim© Parameter	Importance Measure (ranks)	Correlation Coefficient (ranks)	Regression Coefficient (ranks)	Partial Coefficient (ranks)
Darcy_Flux_Mult_SZ	0.532	-0.734	-0.707	-0.900
Recharge_Late_PC_Uncert	0.342	0.565	0.561	0.847
Grout_Kd_Uncert[Tc]	0.045	-0.229	-0.180	-0.458
Grout_Diff_Coeff_Uncert	0.035	0.072	0.104	0.279

GoldSim© simulation software is copyrighted by GoldSim Technology Group LLC of Issaquah, Washington (see http://www.goldsim.com).

A discussion of these results is provided.

7.6.1.2 Importance Measure

Using the Importance Measure using ranks, the two most importance parameters contributing to the uncertainty in the peak total groundwater dose from A Farm are related to the saturated zone Darcy flux and the recharge rate under a degraded surface barrier. The Darcy flux in the saturated zone is directly related to the amount of dispersion and dilution that occurs in the

saturated zone once the radionuclides are transported to the water table and extracted for use in a domestic well. Higher Darcy flux values result in greater dispersion and dilution, which leads to lower groundwater concentrations and lower doses when using the contaminated groundwater. The late time recharge rate affects flow in the vadose zone and higher recharge rates result in faster travel times to the point of compliance once radionuclides are released to the vadose zone. Faster travel times result in more vertical spreading of the releases as the radionuclides are transported downward to the water table. Transporting the center of mass to the water table faster results in higher concentrations reaching the groundwater, leading to higher groundwater concentrations and greater doses when consuming the contaminated groundwater. All other parameters had an Importance Measure less than 0.05. When using raw values instead of ranks, these two were two of the top three important parameters.

7.6.1.3 Correlation Coefficients

The three most important parameters describing the range of values for the peak total groundwater dose from A Farm using the rank correlation coefficients include the two parameters identified using the Importance Measure and the distribution coefficient (K_d) for ^{99}Tc sorption onto grout. The ^{99}Tc K_d is used to transport ^{99}Tc through the grouted base of the tank. Higher values result in greater sorption to the grout, which retards ^{99}Tc movement through the base mat, which reduces the ^{99}Tc releases to the vadose zone, and ultimately leads to lower doses. Both the Darcy flux parameter and the ^{99}Tc K_d showed strong negative correlations; as the values increase, the doses decrease. The late recharge rate had a strong positive correlation; as the recharge rate increases, the dose increases. Given that ^{99}Tc is one of the primary dose contributors to the total dose, it is expected that parameters affecting ^{99}Tc migration to the water table would strongly affect the dose result. When using raw values instead of ranks, the distribution coefficient for uranium in sandy sediments shows up as the next most important parameter affecting the total groundwater dose from A Farm. Like the distribution coefficient for ^{99}Tc, the correlation is negative. Given that uranium is the next highest contributor to dose, it was also expected that parameters pertaining to uranium migration to the water table would strongly affect the dose result.

7.6.1.4 Standardized Regression Coefficients

The four most important parameters describing the range of values for the peak total groundwater dose from A Farm using the standardized regression coefficient include the three parameters identified using the correlation coefficients and the grout diffusivity. The grout diffusivity is related to how fast radionuclides can diffuse through the base mat into the vadose zone. The positive correlation coefficient is consistent with the physical phenomena that higher diffusivity values yield faster diffusion rates. Faster diffusion rates will result in greater releases from the source term into the vadose zone, which would ultimately lead to higher doses from the groundwater pathway.

7.6.1.5 Partial Correlation Coefficients

The four most important parameters describing the range of values for the peak total groundwater dose from A Farm using the partial correlation coefficient method are the same parameters that were determined to be important using the Standardized Regression Coefficient method.

7.6.1.6 Additional Discussion

The importance analysis was repeated for selected metrics to provide confidence that the model results are consistent with the conceptual and mathematical models used for simulating tank releases that ultimately would result in a dose to a member of the public in the future. The analysis was focused at explaining the dose result and not so much at explaining why a certain radionuclide does not contribute significantly to a dose result.

The importance analysis was repeated for the peak total groundwater dose from AX Farm sources. Although the value of the Importance Measure differed, Darcy_Flux_Mult_SZ and Recharge_Late_PC_Uncert were identified as the uncertain parameters with the greatest effect on the uncertainty in the AX Farm total groundwater dose. The other two parameters in Table 7-2, Grout_Diff_Coeff_Uncert and Grout_Kd_Uncert[Tc], were identified as the next most important parameters. Using the Partial Rank Coefficient method, these same four parameters were the most important parameters affecting AX Farm dose uncertainty.

The importance analysis was repeated for the ^{99}Tc groundwater dose from A Farm sources. The same four parameters that were important for characterizing the uncertainty in the total dose from A Farm source were identified as the four key parameters most affecting the uncertainty in the ^{99}Tc dose from all A Farm sources. In addition, the K_d for ^{99}Tc sorption onto the sandy sediments underneath A Farm was identified as the fifth most important parameter. Since ^{99}Tc is the primary dose contributor to the total groundwater dose, it is expected that the same parameters are important to characterizing the uncertainty in both metrics.

The importance analysis was repeated for the ^{233}U groundwater dose from A Farm sources. The Importance Measure method and partial rank coefficient methods both identified the K_d of uranium to sand and the late recharge rates as the key parameters. From Figure 7-17and

Figure 7-22, it is observed that the groundwater dose from ^{233}U from A Farm sources is dominated by the releases from the non-tank sources. Releases into the vadose zone from non-tank sources are controlled by advection and have very little uncertainty. Therefore, the lack of correlation between ^{233}U dose and diffusion parameters is consistent with the release behavior of the key source. Furthermore, the correlation to two parameters that are used in the vadose zone transport model is also consistent with expectations since very little uncertainty in the source term releases was observed.

The importance analysis was repeated for the cumulative release of ^{99}Tc from A Farm tanks in 10,000 years (see Figure 7-15). The Importance Measure and partial rank coefficient methods identify the late time recharge rate, grout diffusivity and grout K_d for ^{99}Tc to be the most important parameters affecting the uncertainty in the cumulative ^{99}Tc release from the A Farm tanks over 10,000 years. This result is consistent with the release model from the A Farm tanks, which is a diffusion release model with limited advection into the top of the vadose zone due to the tank shadow.

The importance analysis was repeated for the cumulative release of ^{233}U from A Farm tanks in 10,000 years (see Figure 7-17). The Importance Measure and partial rank coefficient methods identify the grout diffusivity, uranium solubility, grout K_d for uranium, and the late recharge rate to be the most important parameters affecting the uncertainty in the cumulative ^{233}U release from the A Farm tanks over 10,000 years. This result is consistent with the release model from the A Farm tanks, which is a diffusion release model constrained by a solubility limit and has limited advection into the top of the vadose zone due to the tank shadow.

The importance analysis was repeated for the cumulative release of ^{233}U from A Farm non-tanks sources in 10,000 years (see Figure 7-17). The Importance Measure and partial rank coefficient methods identify the uranium solubility, late recharge rate, and sand K_d for ^{237}Np to be the most important parameters affecting the uncertainty in the cumulative ^{233}U release from these sources over 10,000 years. This result is consistent with the release model from the A Farm non-tank sources, which is an advection release model constrained by a solubility limit and has an inventory source from radionuclide decay of ^{237}Np. The higher the K_d for ^{237}Np in the soils surrounding the pipelines, the less mobile it is and the more likely it will decay to ^{233}U before reaching the vadose zone.

7.6.2 Importance Analysis Corroboration

While performing the importance analysis described in Section 7.6.1, occasionally one method identified an important parameter that was not identified by the other methods and was not expected to be correlated to the output result. For instance, the correlation coefficient method identified the K_d for radium and americium to sand to be more important than the K_d for technetium to sand but the partial Rank Correlation method identified this as one of the most important parameters. Although chemical interactions and competitive sorption can affect transport processes in the natural system, the system model does not account for these competitive transport processes so the K_d of radium and americium should not impact the ^{99}Tc dose from the groundwater pathway. The correlation between these inputs and output is considered spurious. Relationships that are considered spurious, based on knowledge of the fate

and transport models, were used to identity when an importance analysis truly identified a strong correlation between the inputs and the outputs.

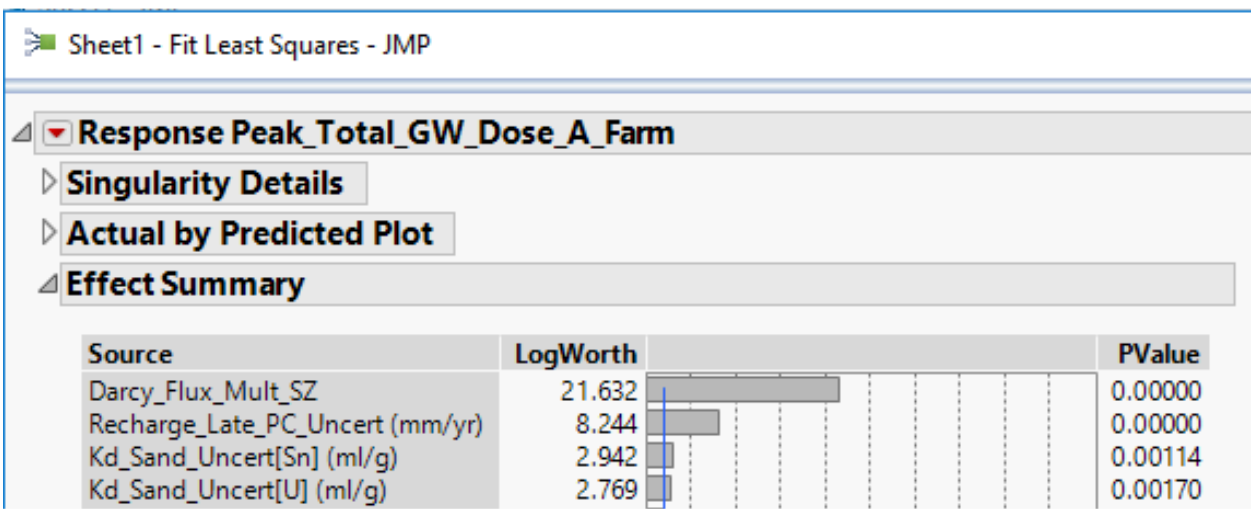
To corroborate the results exported by GoldSim©, two additional methods for importance analyses were performed.

7.6.2.1 Least Squares Effect Screening

JMP version 13 software was used to corroborate the results generated by GoldSim© sensitivity analysis. The importance analysis method used a least squares effect screening to calculate a p-value, which is used to identify the strength of the correlation between the input parameter and the output result. Generally p-values below 0.005 are considered a significant correlation.

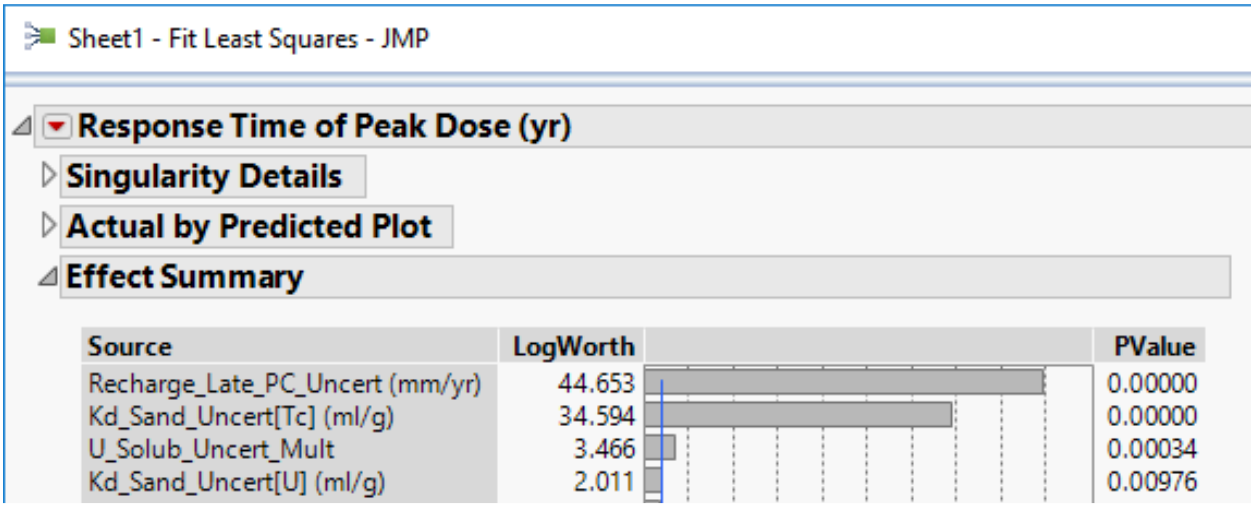
When all of the uncertain input parameters were used in an analysis of peak total groundwater dose from A Farm sources, the parameters that had p-values lower than 0.005 (see Figure 7-24) were Darcy_Flux_Mult_SZ, Recharge_Late_PC_Uncert, Kd_Sand_Uncert[Sn], and Kd_Sand_Uncert[U]. The p-values for Darcy_Flux_Mult_SZ and Recharge_Late_PC_Uncert were well below 0.005, indicating a strong correlation to these parameters. The p-values for the other two were below 0.005, but much higher than the values for Darcy_Flux_Mult_SZ and Recharge_Late_PC_Uncert.

Figure 7-24. Importance Analysis for Peak Total Dose from 241-A Tank Farm Sources.



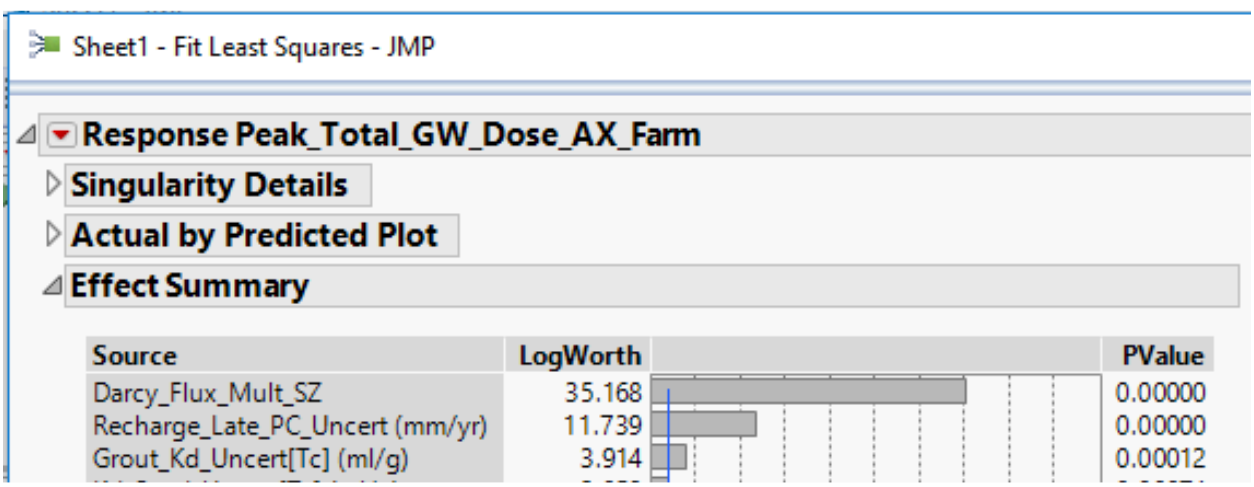
When all of the uncertain input parameters were used in an analysis of time of the peak total groundwater dose from A Farm sources, the parameters that had p-values lower than 0.005 (see Figure 7-25) were Recharge_Late_PC_Uncert, Kd_Sand_Uncert[Tc], andU_Solub_Uncert_Mult. The recharge rate and K_d for ^{99}Tc in the Hanford sands affect how fast ^{99}Tc migrates to the groundwater and then to the point of exposure. The uncertainty on the solubility of uranium is influential on the time of the peak dose because it determines whether the peak is driven by ^{99}Tc or ^{233}U. Uranium has a higher K_d to the Hanford sands and arrives at the water table after ^{99}Tc. If the solubility of uranium is high enough, then the dose from uranium can be higher than the dose from ^{99}Tc, which together lead to later times for the peaks.

Figure 7-25. Importance Analysis for Time of Peak Total Dose from 241-A Tank Farm Sources.



When all of the uncertain input parameters were used in an analysis of peak total groundwater dose from AX Farm sources, the parameters that had p-values lower than 0.005 (see Figure 7-26) were Darcy_Flux_Mult_SZ, Recharge_Late_PC_Uncert, and Grout_Kd_Uncert[Tc]. This result corroborates the GoldSim© importance analysis.

Figure 7-26. Importance Analysis for Peak Total Dose from 241-AX Tank Farm Sources.

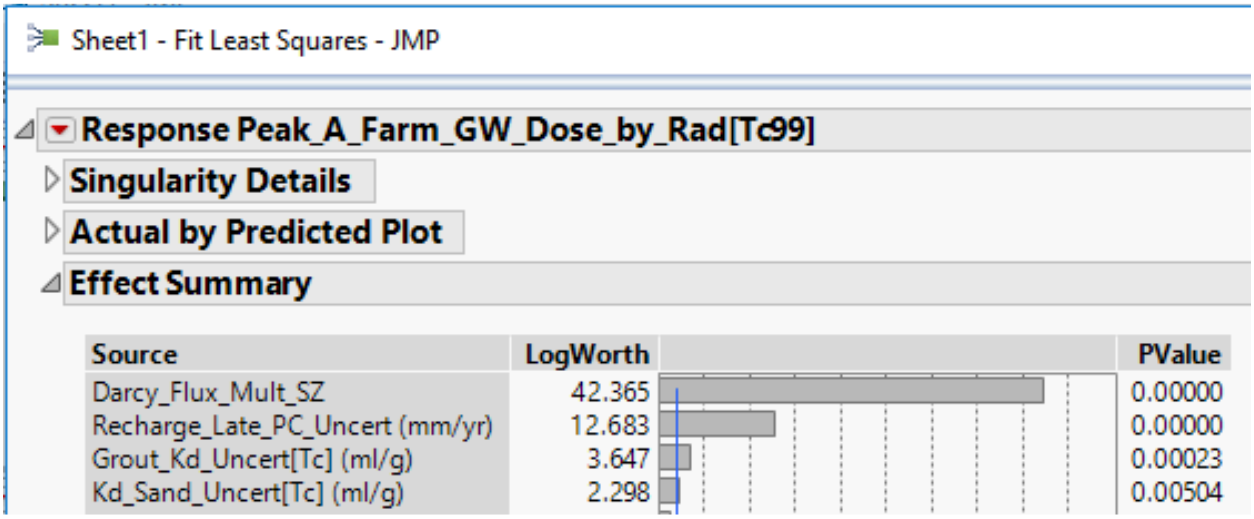


When all of the uncertain input parameters were used in an analysis of time of the peak total groundwater dose from AX Farm sources, the important parameters for characterizing the range of values for the time of the peak dose from AX Farm were the same as those that affect the time of the peak dose from A Farm.

When all of the uncertain input parameters were used in an analysis of peak ^{99}Tc groundwater dose from A Farm sources, the parameters that had p-values lower than 0.005 (see Figure 7-27)

were Darcy_Flux_Mult_SZ, Recharge_Late_PC_Uncert, and Grout_Kd_Uncert[Tc]. This result corroborates the GoldSim© importance analysis.

Figure 7-27. Importance Analysis for Peak Technetium-99 Dose from 241-A Tank Farm Sources.



When all of the uncertain input parameters were used in an analysis of the cumulative release of ^{99}Tc in 10,000 years to the vadose zone from A Farm tanks, the parameters that had p-values lower than 0.005 (see
Figure 7-28) were Recharge_Late_PC_Uncert, Grout_Kd_Uncert[Tc], and Grout_Diff_Coeff_Uncert. Figure 7-29 is a graphical illustration of how strongly correlated the output is to these inputs; the cumulative release can almost be calculated using a linear representation of just these three variables. This result corroborates the GoldSim© importance analysis.

When all of the uncertain input parameters were used in an analysis of the cumulative release of ^{99}Tc in 10,000 years to the saturated zone from A Farm tanks, the parameters that had p-values lower than 0.005 (see Figure 7-30) were the same as those that affect the range of values for the release to the vadose zone, but also include the K_d for ^{99}Tc onto vadose zone sediments (Kd_Sand_Uncert[Tc]). Figure 7-31 is a graphical illustration of how strongly correlated the output is to these inputs; the cumulative release can almost be calculated using a linear representation of just these four variables. Note how the K_d for ^{99}Tc in sand is added as a color. Blue-colored dots represent lower K_d values and red-colored dots represent higher K_d values. Within each box, whose points have similar ranges of the other three parameters, the blue dots tend to have higher cumulative releases than grey- or red-colored markers. This result corroborates the GoldSim© importance analysis.

Figure 7-28. Importance Analysis for Cumulative Release of Technetium-99 to Vadose Zone from 241-A Farm Tanks.

Sheet1 - Fit Least Squares - JMP

Response A_Tanks_to_VZ[Tc99]

Singularity Details

Actual by Predicted Plot

Effect Summary

Source	LogWorth	PValue
Recharge_Late_PC_Uncert (mm/yr)	105.990	0.00000
Grout_Kd_Uncert[Tc] (ml/g)	74.363	0.00000
Grout_Diff_Coeff_Uncert (cm2/s)	28.316	0.00000

Figure 7-29. Graphical Depiction of Correlation between Key Uncertainties and the Cumulative Release of Technetium-99 to Vadose Zone from 241-A Farm Tanks.

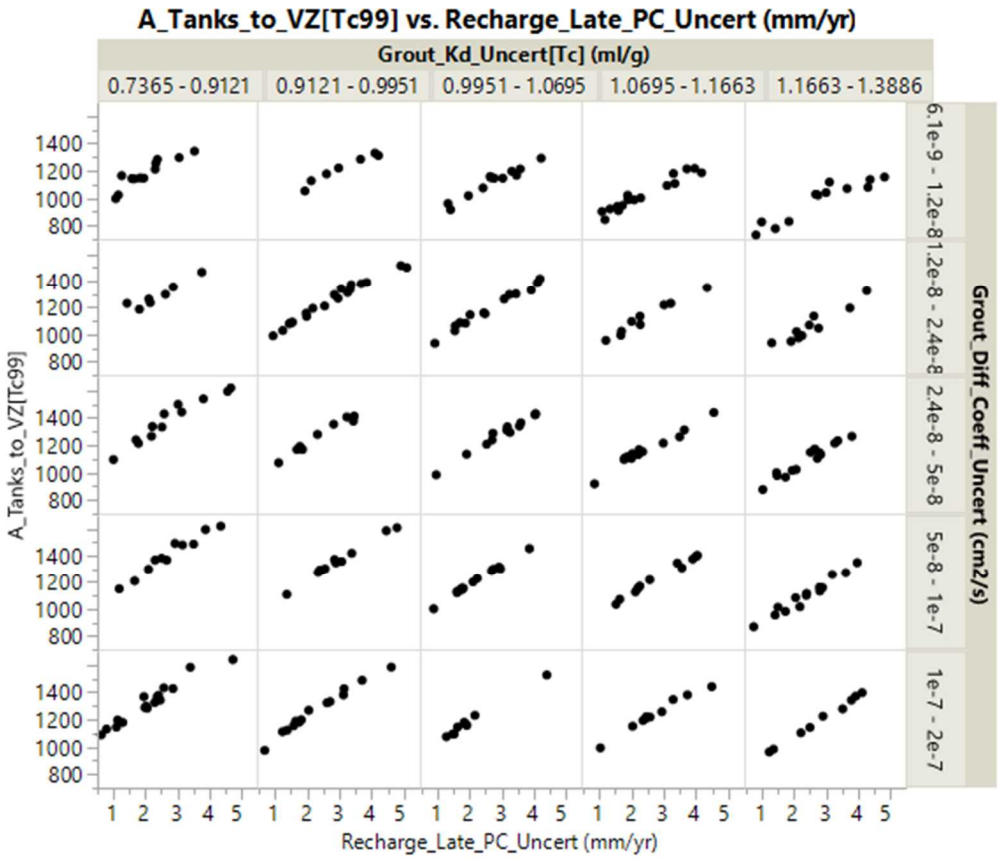
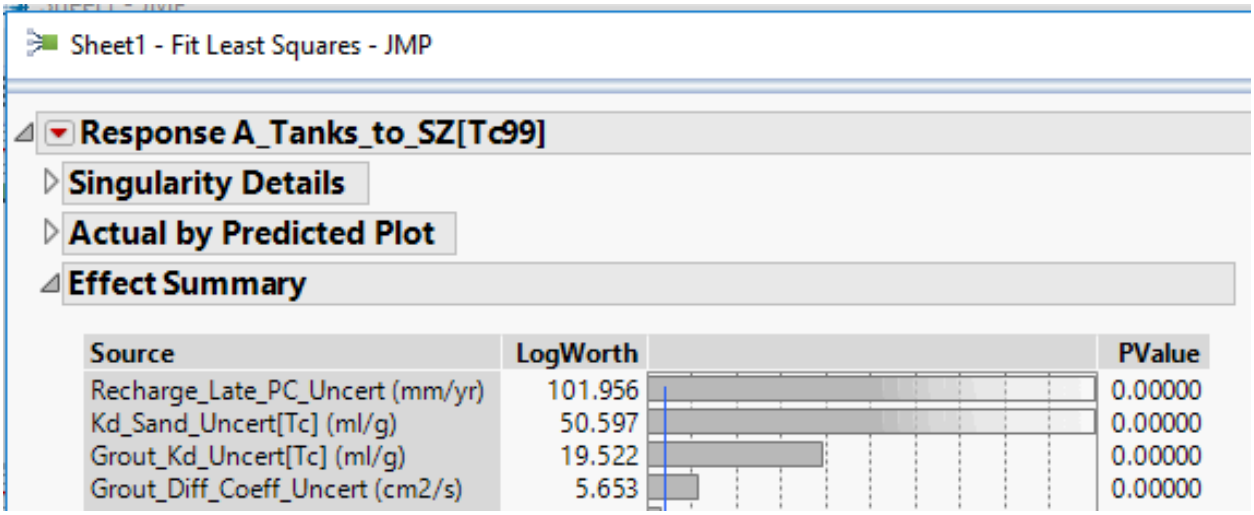
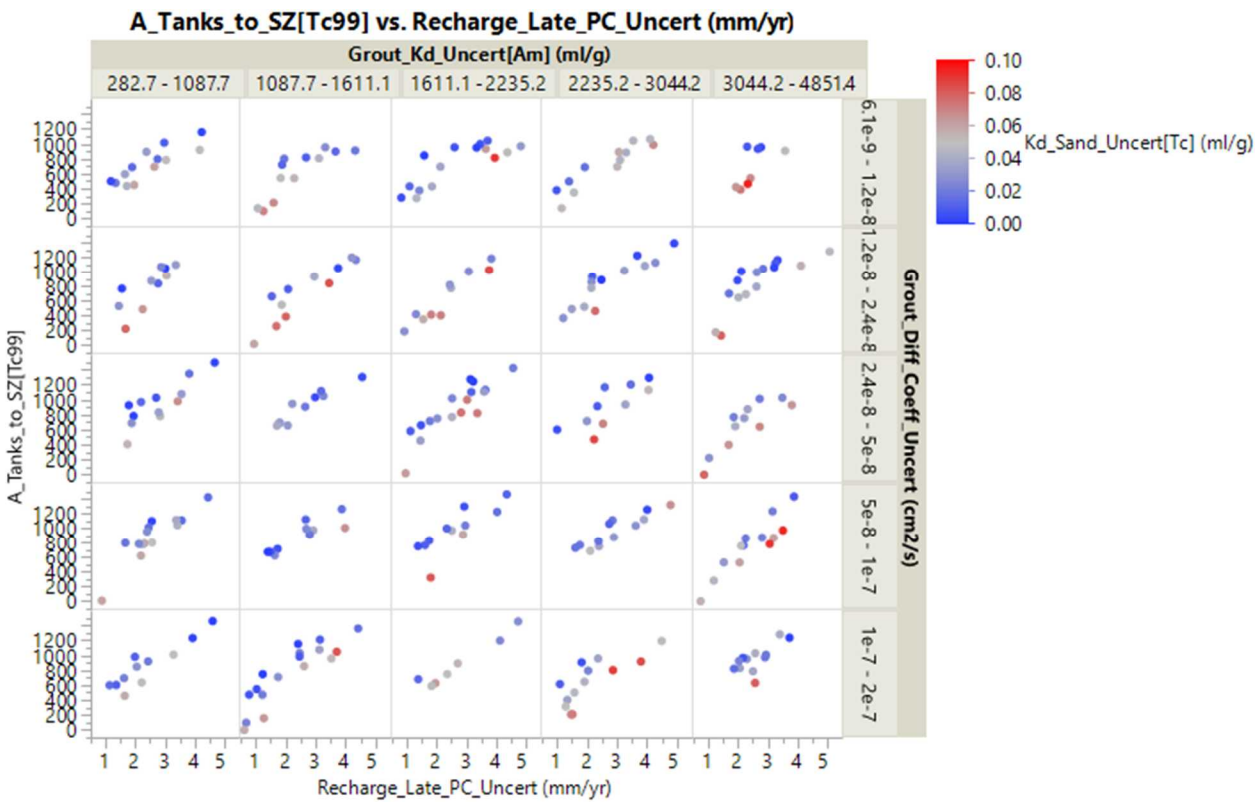


Figure 7-30. Importance Analysis for Cumulative Release of Technetium-99 to Saturated Zone from 241-A Farm Tanks.



Source	LogWorth	PValue
Recharge_Late_PC_Uncert (mm/yr)	101.956	0.00000
Kd_Sand_Uncert[Tc] (ml/g)	50.597	0.00000
Grout_Kd_Uncert[Tc] (ml/g)	19.522	0.00000
Grout_Diff_Coeff_Uncert (cm2/s)	5.653	0.00000

Figure 7-31. Graphical Depiction of Correlation between Key Uncertainties and the Cumulative Release of Technetium-99 to Saturated Zone from 241-A Farm Tanks.



7.6.2.2 Random Forest Method

The Random Forest method was used to corroborate the importance analysis results presented in Section 7.6. The algorithm used in the importance analysis is the Random Forest algorithm originally developed by Leo Breiman (Brieman 2001). The Random Forest algorithm is machine learning algorithm based on decision tree analysis (Brieman 2001). A random subsample of the input data set (i.e., sampled values from the uncertainty distributions in each realization of the Monte Carlo analysis) is drawn together with the model output result. The resulting dataset is the model training data set. The number of predictors used in the training data set is a fraction of the entire dataset. A general rule of thumb for determining the number of predictors to include in the subsample is to select an integer value that is approximately equal to the square root of the number of total predictors. A decision tree analysis is performed with this first subset to find the splitting condition that generates the best prediction of the output. For a continuous outcome, such as a PA model output, the splitting condition is a regression model to the target variable using each of the independent predictor variables (one at a time). The sum of squared errors (SSE) between the regression model prediction and the output is computed at each split point. The variable resulting in the minimum SSE is the predictor selected from the first decision tree node. The data is split into two sets based on the splitting condition. Once the model output is parsed into the separate groups by the first splitting condition, the analysis is repeated on each of these groups. For each group another random draw of predictor inputs is used, not the same

sampling of predictors from the first round. The algorithm repeats the analysis for multiple nodes and multiple trees until as much information as can be learned from the training data is derived. The decision trees developed from the training dataset are tested with the full dataset to evaluate the capability of each tree to predict the outcome. Finally, the resulting predictors are ranked according to propensity to be the parameter most likely to be included in a splitting condition that best predicts the outcome for the full dataset.

A copy of the R-script used to perform the importance analysis is provided in Appendix B.

The results of the analysis are presented in Table 7-3 for the magnitude of the peak total groundwater dose from A Farm and AX Farm sources, as well as the time of the peak total groundwater dose from each tank farm. The %IncMSE is an indicator for the strength of the correlation between the input and the results; higher values mean stronger correlations. The value in parentheses is the numerical ranking of the parameter in the importance analysis result. The lower the value, the higher the %IncMSE for that parameter. The importance analysis results shown in Table 7-3 fully corroborate the results presented in Section 7.6.

A discussion of the results for the A Farm total groundwater dose is provided after the table of results.

For the peak total groundwater dose from all A Farm sources, the random forest method identified Darcy_Flux_Mult_SZ, Recharge_Late_PC_Uncert, and Kd_Sand_Uncert_U as the three most significant parameters that affect the range of values for the total groundwater dose to a member of the public in the future. Partial dependency plots for these three parameters are provided in Figure 7-32.

The partial dependency plots show that Darcy_Flux_Mult_SZ is the most important parameter for describing the uncertainty in the peak total groundwater dose. There is a negative correlation between this parameter and the peak dose; as the saturated zone Darcy flux multiplier value increases, the peak total groundwater dose decreases. Higher multipliers mean faster groundwater velocities and greater dilution of the plume. The positive correlation in the Recharge_Late_PC_Uncert partial dependency plot shows that increasing the recharge rate, which lowers travel times through the vadose zone, results in higher peak doses. The sharp drop in the partial dependency plot for Kd_Sand_Uncert_U suggests that the importance of this parameter may be determined by just a few realizations. It is hypothesized to be due to the strong correlation in just a few realizations that have uranium travel times that make the peak uranium dose higher than the peak ^{99}Tc dose. Uranium is the dominant contributor to the peak total groundwater dose in fewer than 5% of the Monte Carlo realizations.

For the time of the peak total groundwater dose from all A Farm sources, the random forest method identified Recharge_Late_PC_Uncert, Kd_Sand_Uncert_Tc, and Kd_Sand_Uncert_U as the three most significant parameters that affect the range of values for the time of the peak total groundwater dose. Partial dependency plots for these three parameters are provided in Figure 7-33.

The partial dependency plots show that Recharge_Late_PC_Uncert is the most important parameter for describing the uncertainty in the timing of the peak total groundwater dose and that there is a negative correlation. When the recharge rate under a degraded surface barrier increases, the peak dose occurs earlier. Increasing the recharge rate increases flow rates in the vadose zone, which reduces travel times through the vadose zone. The positive correlation in the Kd_Sand_Uncert_Tc partial dependency plot shows that lower K_d values lead to earlier peak groundwater doses. Lower K_d values result in less retardation in the vadose zone and faster vadose zone travel times. The faster the travel times to the saturated zone, the sooner that the peak dose occurs. This correlation is the strongest radionuclide-specific uncertainty because ^{99}Tc is the most significant contributor to the total groundwater dose. The negative correlation shown in the partial dependency plot for Kd_Sand_Uncert_U is opposite of the correlation for ^{99}Tc and is not by itself intuitive. Uranium has a higher K_d than technetium in the vadose zone, so it has longer travel times through the vadose zone such that the dose from uranium is still increasing at the end of the simulation. Uranium drives the peak total groundwater dose in fewer than 5% of the Monte Carlo realizations, but the peak uranium dose is still increasing at the end of the simulation; the peak dose in these realizations also occurs at the end of the simulation. Consequently, the time of the peak dose occurs later, consistent with the shift from technetium driving the peak dose to uranium driving the peak dose. Darcy_Flux_Mult_SZ does not strongly influence the timing of the peak dose because this parameter affects the amount of dilution that occurs in the saturated zone, which affects the magnitude of the dose but not the timing.

Partial dependency plots for the peak total groundwater dose from AX Farm sources and time of the peak dose are similar to the partial dependency plots for A Farm sources.

Table 7-3. Importance Analysis Results using the Random Forest Method.

Parameter	%IncMSE			
	Peak Total Groundwater Dose from 241-A Tank Farm Sources	Time of the Peak Groundwater Dose from 241-A Tank Farm Sources	Peak Total Groundwater Dose from 241-AX Tank Farm Sources	Time of the Peak Groundwater Dose from 241-AX Tank Farm Sources
Darcy_Flux_Mult_SZ	74.96 (1)	0.43 (33)	77.95 (1)	0.76 (29)
Recharge_Late_PC_Uncert	32.79 (2)	124.94 (1)	35.21 (2)	138.36 (1)
Kd_Sand_Uncert_U	32.28 (3)	35.09 (3)	15.07 (3)	29.89 (3)
Grout_Kd_Uncert_Tc	4.92 (5)	104.28 (2)	3.62 (5)	98.02 (2)
Grout_Diff_Coeff_Uncert	4.33 (6)	2.41 (7)	14.05 (4)	1.43 (13)
Values in parentheses represent the rank of the parameter in the importance analysis.				

Figure 7-32. Partial Dependency Plots for Three Uncertain Parameters to the Peak Total Groundwater Dose from 241-A Tank Farm Sources: (a) Darcy_Flux_Mult_SZ, (b) Recharge_Late_PC_Uncert, and (c) Kd_Sand_Uncert_U.

a b c

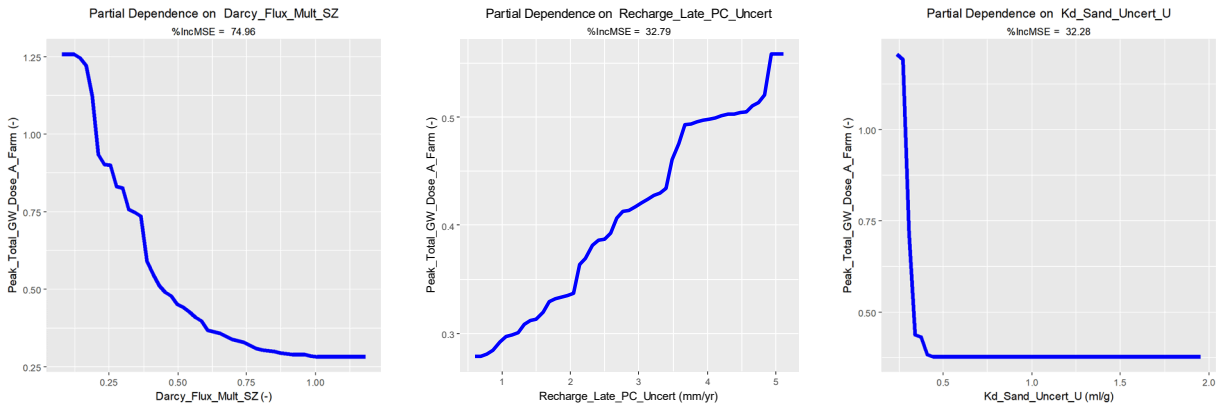
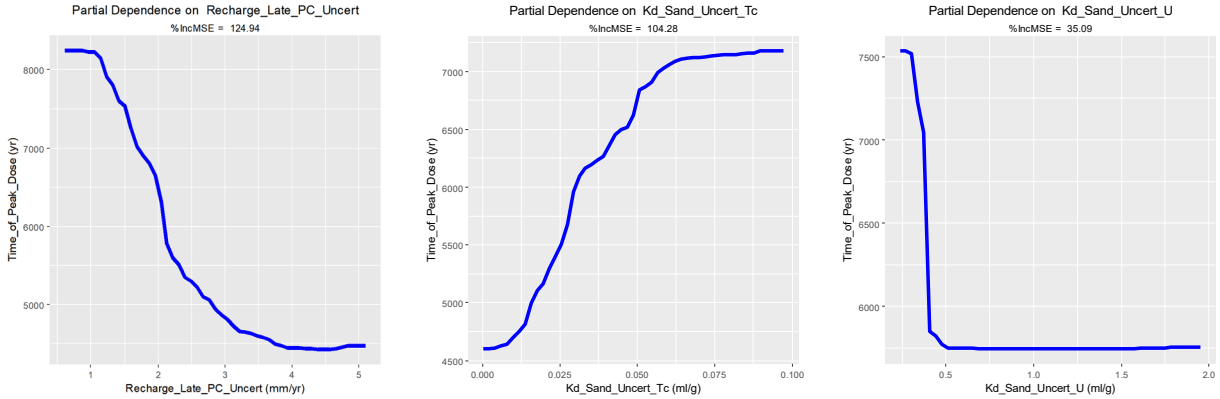


Figure 7-33. Partial Dependency Plots for Three Uncertain Parameters to the Time of the Peak Total Groundwater Dose from 241-A Tank Farm Sources: (a) Recharge_Late_PC_Uncert, (b) Kd_Sand_Uncert_Tc, and (c) Kd_Sand_Uncert_U.

a b c



7.7 SINGLE REALIZATION ANALYSES

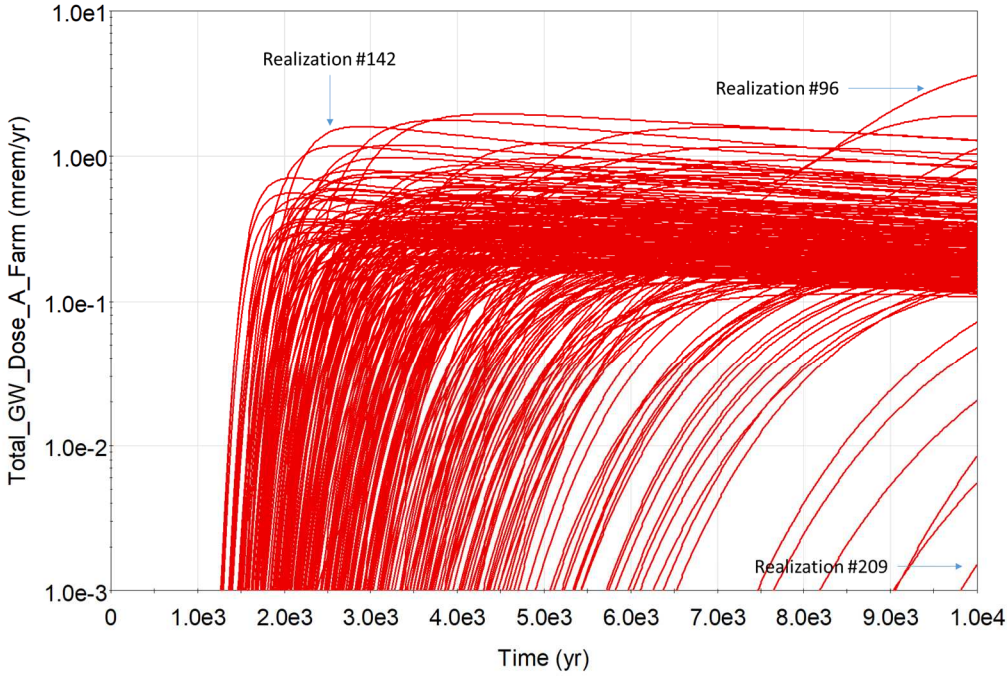
Single realizations from the Monte Carlo uncertainty analysis were investigated to demonstrate an understanding of the model results and corroborate the results of the importance analysis. The metric evaluated was the total groundwater dose originating from sources in the A-Tank Farm. Three realizations were selected, one with the highest peak dose in the 10,000-year simulation (Realization #96), one with a high dose and early breakthrough (Realization #142), and one with a low dose and late breakthrough (Realization #209) (see .Figure 7-34). Figure 7-34a shows the dose histories with all realizations in the Monte Carlo analysis and Figure 7-34b shows the three realizations together with the mean, 5th-percentile, 50th-percentile, and 95th-percentile dose histories.

7.7.1 Analysis of Realization #96

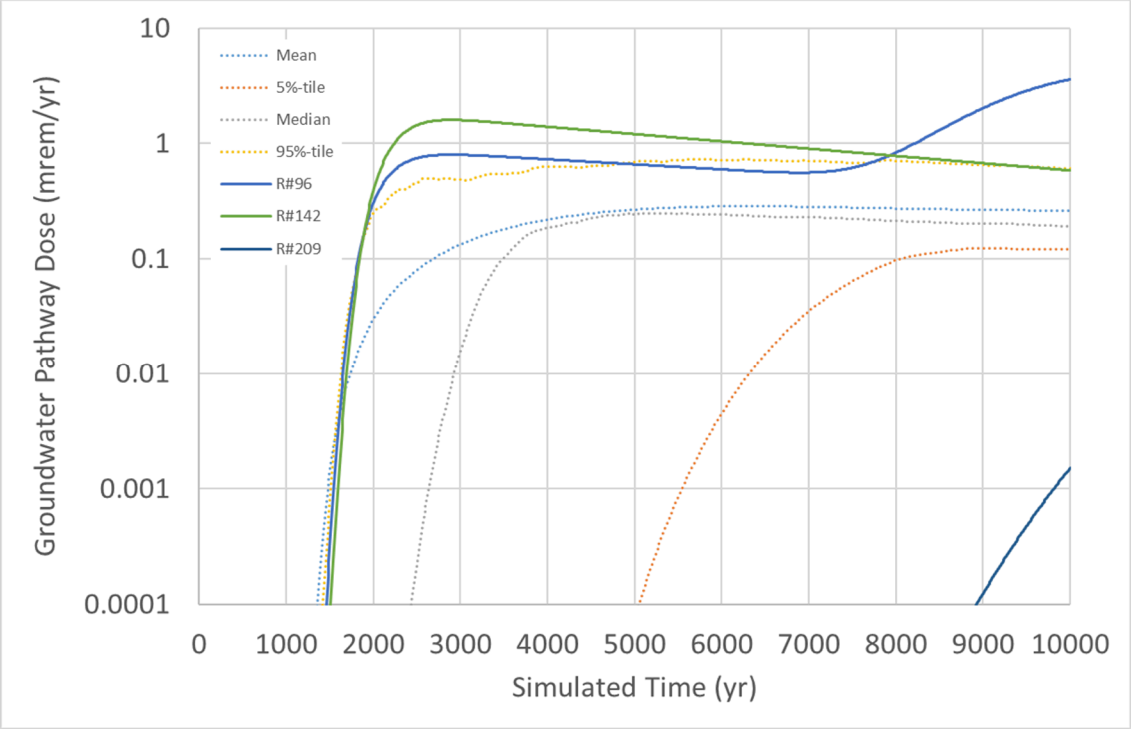
The dose history from A-Farm sources in realization #96 has two peaks, one at early times and one at late times. The early peak is due to ^{99}Tc from tanks A-105 and A-104 and the later peak is due to ^{233}U from the non-tank sources (see Figure 7-35). In Realization #96 the initial ^{99}Tc peak is not the earliest nor the highest ^{99}Tc peak among all realizations (see Figure 7-34a). The sampled net infiltration rate under the degraded surface barrier is 3.33 mm/yr, which is in the 77th-percentile of the distribution. The sampled distribution for ^{99}Tc to grout is 0.98 ml/g, which is in the 36th-percentile of the distribution. The sampled distribution coefficient for ^{99}Tc in the sands of the Hanford formation is 0.0052 ml/g, which is in the 10th-percentile of the distribution. A high net infiltration rate coupled with a low distribution coefficients results in fast release times from the source and fast transport times through the vadose zone that increase vertical spreading in the natural system and result in doses at earlier times. The magnitude of the dose is driven by little dispersion and dilution in the saturated zone due to sampling the saturated zone Darcy flux multiplier (0.33) at the 7th-percentile of the distribution. Low saturated zone Darcy Flux multiplier values represent low hydraulic conductivities of the saturated sediments. The low Darcy flux multiplier will cause low dilution values for all constituents resulting in higher total groundwater doses.

Figure 7-34. Total Groundwater Dose from 241-A Farm (a) All 300 Realizations (b) Selected Single Realizations with Statistics from 300 Realizations.

(a)



(b)

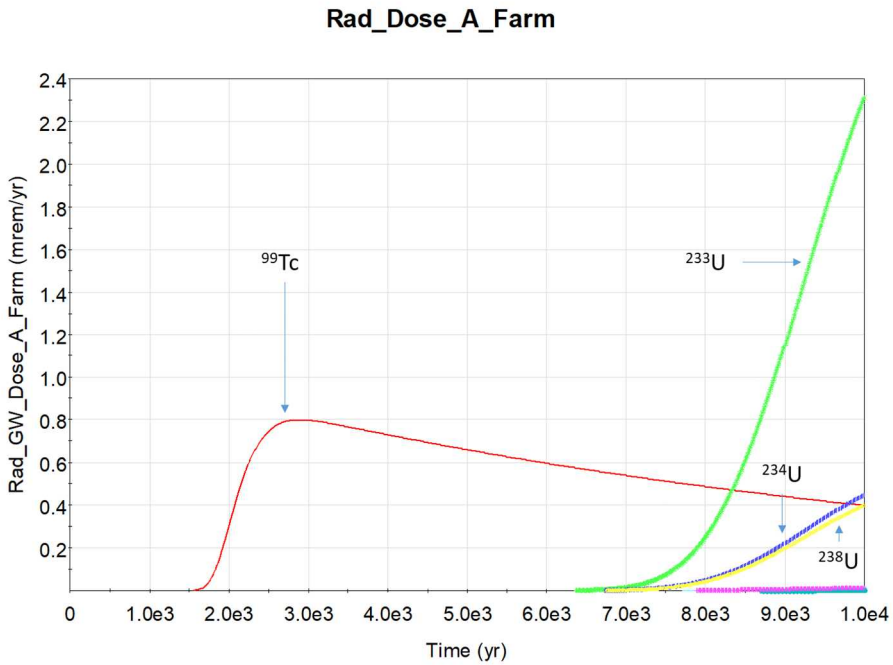


In Realization #96 the initial ^{233}U dose is the highest in any realization and is still increasing at the end of the simulation (see Figure 7-37). The net infiltration rate and low Darcy flux multiplier result in faster mobility and less dispersion and dilution of all radionuclides. The distribution coefficient for uranium onto grout is sampled at the 93rd percentile (2515.75 ml/g). Sampling a high distribution coefficient for the grout would be expected to limit uranium releases from the sources. However, the ^{233}U dose from A Farm is driven by the non-tank sources (i.e., pipelines), which are not grouted in the PA. Therefore, a high grout distribution coefficient for uranium does not influence the uranium dose significantly. However, the distribution coefficient for uranium in the Hanford sands is 0.25 ml/g, which is in the lowest percentile of the distribution (0.004%). As shown in Figure 7-37, very few realizations have any uranium reaching the groundwater so sampling a very low value of the distribution coefficient is necessary for a uranium to reach the groundwater. Even at a sampled value of 0.25 ml/g, the dose curve from ^{233}U is still increasing at the end of the simulation, which demonstrates that transport through the vadose zone is significantly delayed by even small distribution coefficients. A high net infiltration rate coupled with a low distribution coefficient for sands results in fast transport times through the vadose zone that increase vertical spreading in the natural system and result in doses sooner than if values at the other ends of the distributions were selected. The magnitude of the dose is driven by little dispersion and dilution in the saturated zone due to sampling the saturated zone Darcy flux multiplier (0.33) at the 7th-percentile of the distribution. Low saturated zone Darcy Flux multiplier values represent low hydraulic conductivities of the saturated sediments. The low Darcy flux multiplier will cause low dispersion and low dilution for all constituents resulting in higher total groundwater doses. In addition, the solubility uncertainty multiplier for uranium is 0.65, which is in the 19th-percentile of the distribution. The relationship between a low uranium solubility and a high uranium dose contradicts expectations. A lower uranium solubility would be expected to limit releases from the source, leading to concentrations in the natural environment and lower doses. However, the uranium dose is primarily from the non-tank sources. Releases from the non-tank sources are dominated by advection, rather than by diffusion. Solubility in not a significant source release factor when large infiltration rates flow through the source term. This is evident in Figure 7-17b, which shows that nearly all of the ^{233}U inventory is released from the non-tank sources in A-Farm to the vadose zone over a short period of time.

Regarding other radionuclides that do not drive the dose in this realization or any others. The distributions coefficients for technetium and uranium are both below 0.3 ml/g in Realization #96. At 0.25 ml/g, uranium breakthrough to the water table is delayed and releases that occurred in the first few thousand years (see Figure 7-17b) are still being transported through the natural system near the end of the simulation (see Figure 7-37). This provides insight that radionuclides with a distribution coefficient much greater than 0.3 ml/g are sufficiently retarded in the vadose zone, even under the larger recharge rates considered, that they do not reach the water table. Only cobalt, tritium, iodine, niobium, radon, selenium, and technetium have best-estimate distribution coefficients that are lower than 0.3 ml/g. The range for uranium, iodine, and selenium extend up to 2 ml/g or more. Consequently, in many realizations only a few radionuclide would be expected to reach the water table and cause a dose. Furthermore, the half-lives of cobalt, tritium, niobium, and radon are so short that these radionuclides decay before reaching the water table despite the possibly to have low distribution coefficients in the vadose zone.

Figure 7-35. Realization #96 Groundwater Dose from 241-A Farm (a) By Radionuclide (b) By Source.

(a)



(b)

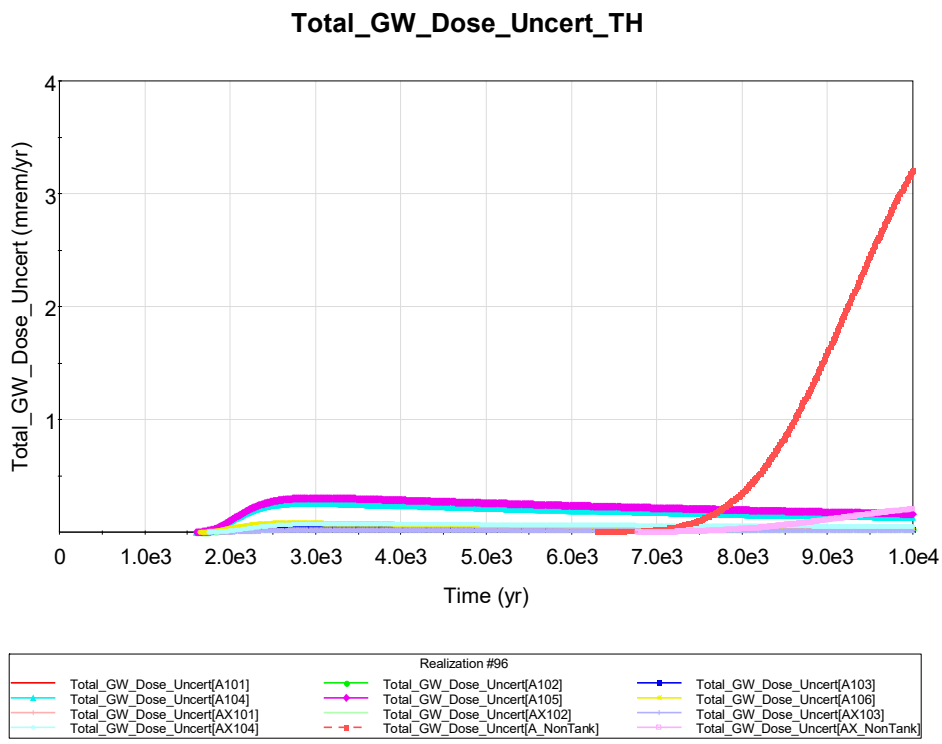


Figure 7-36. Technetium-99 Groundwater Dose from All 241-A Farm Sources, 300 Realizations of Results.

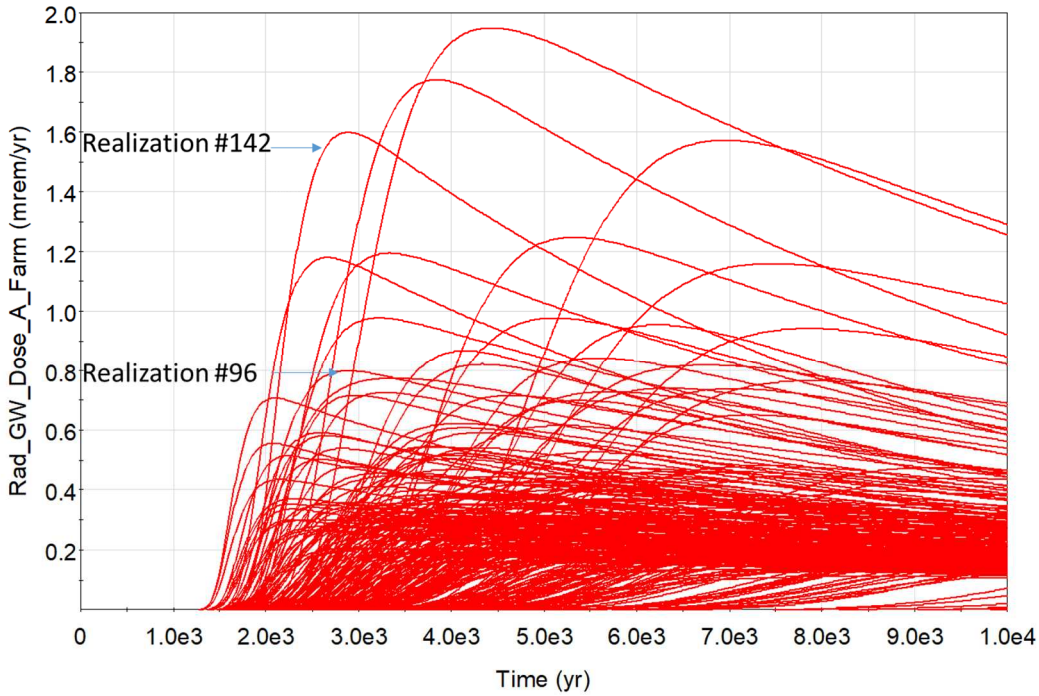
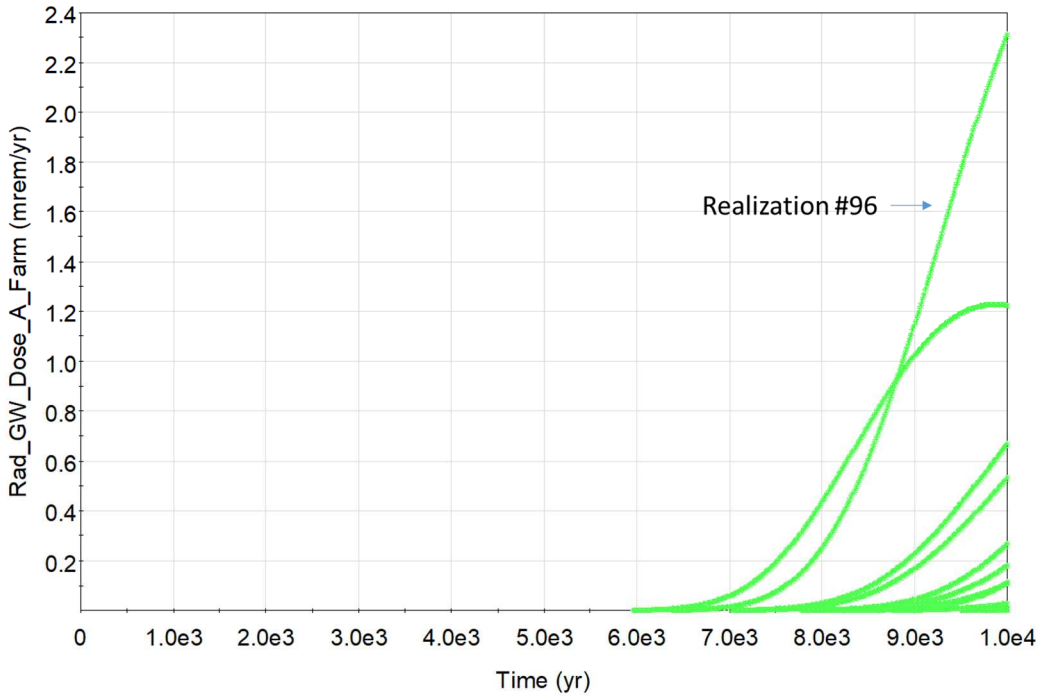


Figure 7-37. Uranium-233 Groundwater Dose from All 241-A Farm Sources, 300 Realizations of Results.



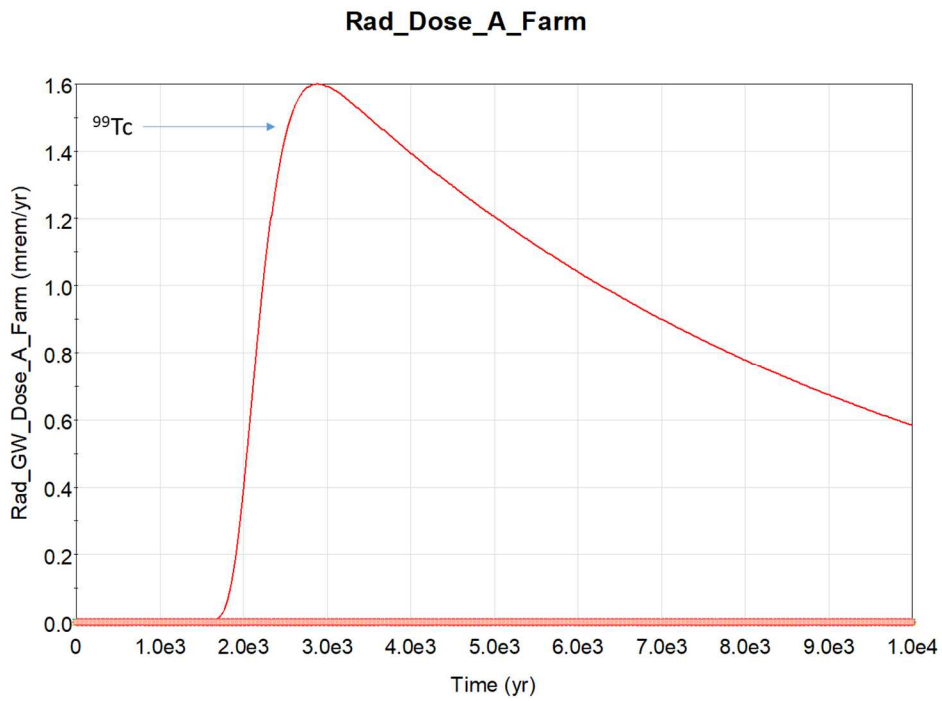
7.7.2 Analysis of Realization #142

Similar to Realization #96, the early dose history from A-Farm sources in realization #142 is due to ^{99}Tc from tanks A-105 and A-104 (see Figure 7-38). Unlike Realization #96, there is no rise in the dose result from ^{233}U originating from the non-tank sources; the dose at all times is primarily from ^{99}Tc from tanks A-105 and A-104. In Realization #142 the initial ^{99}Tc peak is not the earliest nor the highest ^{99}Tc peak among all realizations (see Figure 7-36). The sampled net infiltration rate under the degraded surface barrier is 4.75 mm/yr, which is in the 98th-percentile of the distribution. The sampled distribution for ^{99}Tc to grout is 0.90 ml/g, which is in the 18th-percentile of the distribution. The sampled distribution coefficient for ^{99}Tc in the sands of the Hanford formation is 0.028 ml/g, which is in the 48th-percentile of the distribution. A high net infiltration rate coupled with low distribution coefficients results in fast release times from the source and fast transport times through the vadose zone. Fast transport times through the vadose zone increase vertical spreading in the natural system and result in doses at early time. The magnitude of the dose is driven by dispersion and dilution in the natural system. There is little dispersion and dilution in the saturated zone due to sampling the saturated zone Darcy flux multiplier (0.24) at the 3rd-percentile of the distribution. Low saturated zone Darcy Flux multiplier values represent low hydraulic conductivities of the saturated sediments. The low Darcy flux multiplier will cause low dispersion and low dilution for all constituents resulting in higher total groundwater doses.

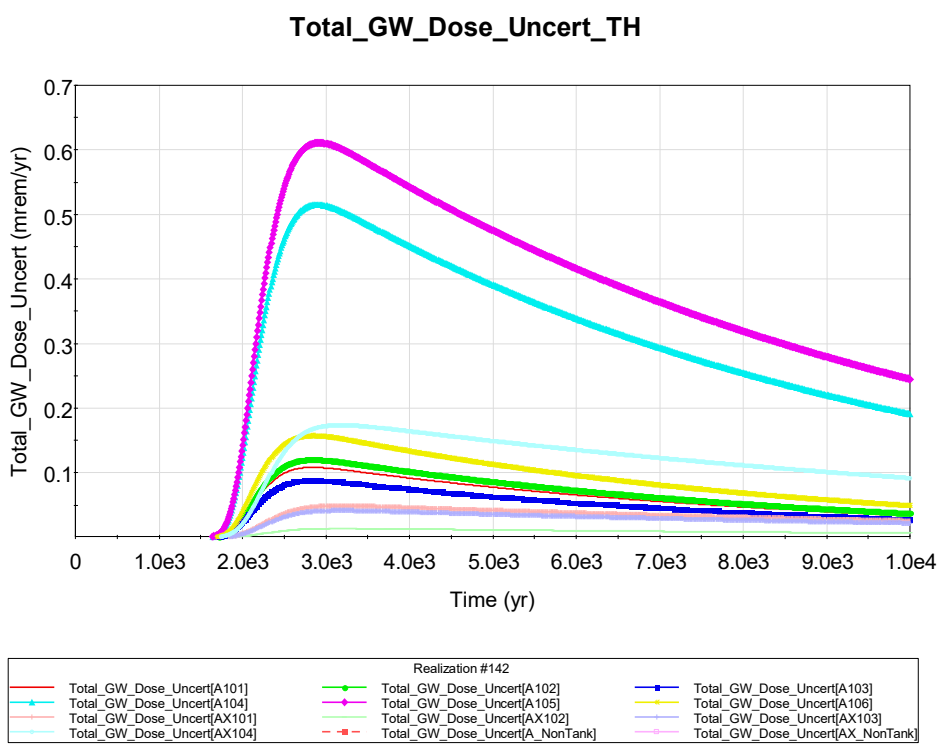
The ^{99}Tc doses in Realizations #96 and #142 are fairly similar, and the sampled parameter values that affect ^{99}Tc mobility from the sources and through the natural environment are also similar. The doses from ^{233}U are not similar in these two realizations. Compared to Realization #96, the net infiltration rate is higher and the Darcy flux multiplier is lower in Realization #142. As a result, uranium transport through the vadose zone and dilution and dispersion in the saturated zone could be expected to cause higher doses in Realization #142. However, this is not the case. There is another controlling parameter that prevents uranium from reaching the groundwater in Realization #142. The sampled value for the distribution coefficient onto the Hanford sands in Realization #142 is 1.18 ml/g, which is at the 73rd percentile of the distribution. Contrast this with the sampled value in Realization #96, which was 0.25 ml/g. In realization #96 the uranium from the non-tank sources had only recently arrived at the point of calculation prior to the simulation end time (see Figure 7-37). In Realization #142 retardation in the vadose zone due to the higher distribution coefficient is enough to prevent uranium from reaching the water table and causing a dose.

Figure 7-38. Realization #142 Groundwater Dose from 241-A Farm (a) By Radionuclide (b) By Source.

(a)



(b)



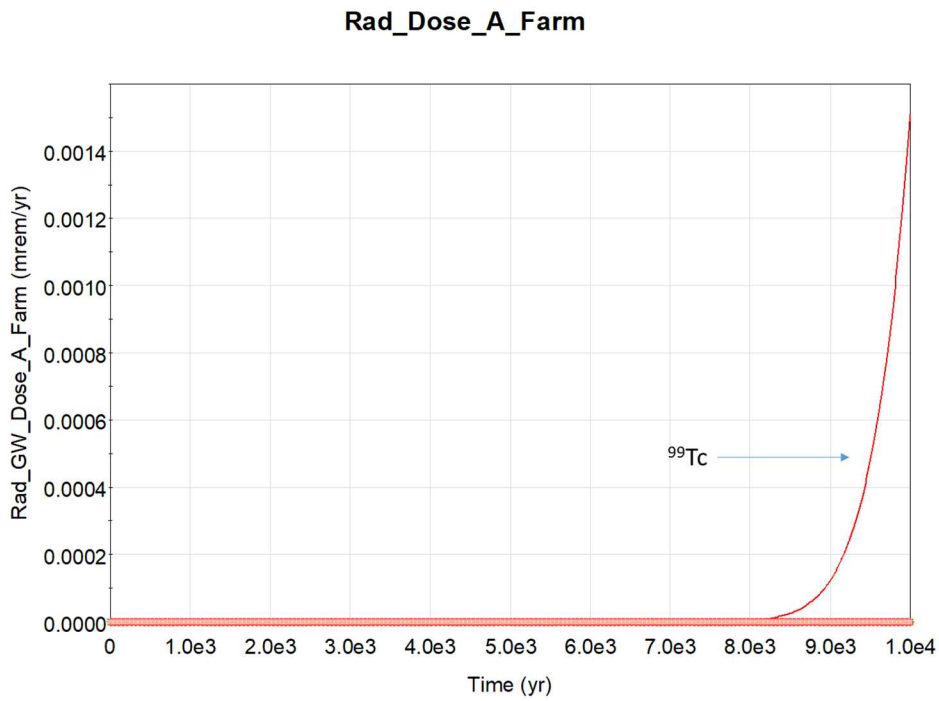
7.7.3 Analysis of Realization #209

The dose in Realization #209, is among the latest to occur and lowest to occur (see Figure 7-36). Like Realization #96 and #142, the dose history from A-Farm sources in realization #209 is due to ^{99}Tc from tanks A-105 and A-104 (see Figure 7-39). Similar to Realization #142, there is no rise in the dose result from ^{233}U originating from the non-tank sources; the dose at all times is primarily from ^{99}Tc from tanks A-105 and A-104. In Realization #209, the sampled net infiltration rate under the degraded surface barrier is 0.62 mm/yr, which is the lowest in the 300 realizations and is sampled below the 1st-percentile value in the distribution. The low net infiltration rate provides very little driving force to move contaminants released from the source terms to the water table. The sampled distribution for ^{99}Tc to grout is 0.79 ml/g, which is in the 3rd-percentile of the distribution. The sampled distribution coefficient for ^{99}Tc in the sands of the Hanford formation is 0.057 ml/g, which is in the 81st-percentile of the distribution. The low net infiltration rate coupled with a high distribution coefficient to the vadose zone sediments limits ^{99}Tc mobility to the groundwater resulting in delayed doses that are still increasing at the end of the simulation. The magnitude of the dose is driven by little dilution and dispersion in the saturated zone due to sampling the saturated zone Darcy flux multiplier (0.33) at the 7th-percentile of the distribution. Although there is little dilution, the dose is still among the lowest because the mobility of ^{99}Tc is limited by the low net infiltration rate and high distribution coefficient in the vadose zone.

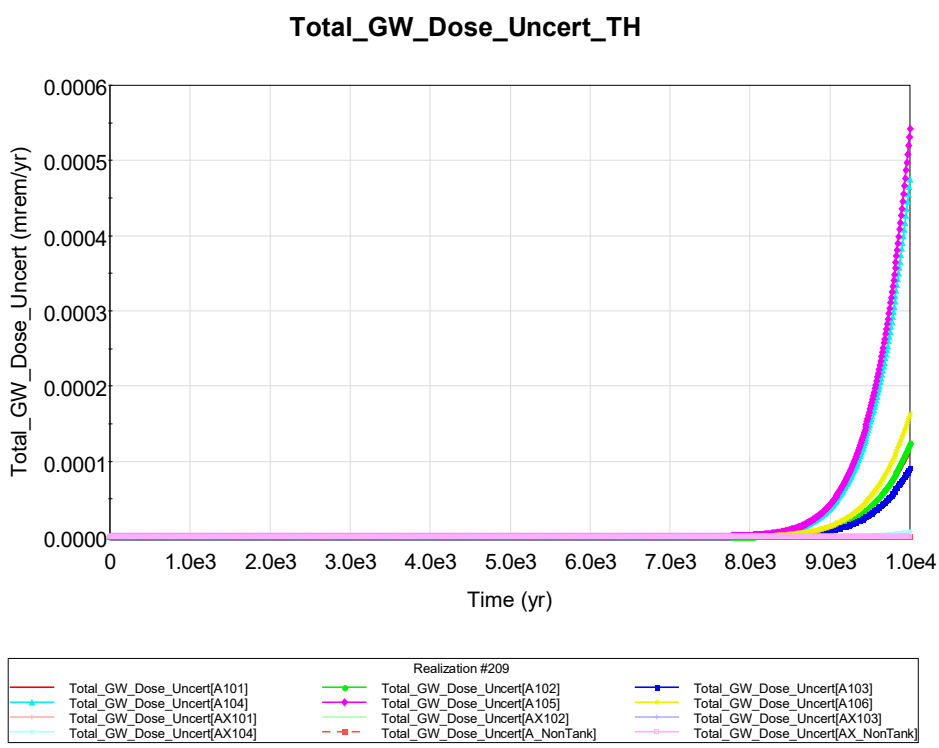
The doses from ^{233}U are low primarily due to the low net infiltration rate coupled with a high distribution coefficient to the vadose zone sediments. In realization #209 the sampled value for the uranium distribution coefficient onto the Hanford sands is 1.27 ml/g, which is at the 79th percentile of the distribution. In Realization #209 retardation in the vadose zone due to the high distribution coefficient is enough to prevent uranium from reaching the water table and causing a dose.

Figure 7-39. Realization #209 Groundwater Dose from 241-A Farm (a) By Radionuclide (b) By Source.

(a)



(b)



7.8 CONCLUSIONS

The uncertainty analysis demonstrates that releases from WMA A-AX after closure of the area will not exceed DOE performance objectives in 1,000 or 10,000 years. The peak groundwater pathway dose in 1,000 years is below 1×10^{-6} mrem/yr, compared to DOE's performance objective of 25 mrem/yr. When uncertainties are considered, the peak dose during the time of compliance is still below 1×10^{-6} mrem/yr. In addition, the peak dose in 10,000 years for any combination of uncertain parameters is 3.6 mrem/yr, which is also below the performance objective for All-Pathways dose.

Furthermore, the uncertainty analysis indicates that there is a very low probability that peak impacts to the groundwater and peak doses could move within the 1,000-year compliance period.

The uncertainty analysis reveals that ^{99}Tc and uranium are the primary dose drivers in 10,000 years. The parameters that most strongly affect the uncertainty in dose results affect the amount of dilution in the saturated zone and the parameters that affect releases of ^{99}Tc and uranium from the tanks and then transport the released mass to the water table. The uncertainty analysis did not investigate inventory uncertainty or uncertainty in the exposure factors, which tend to have proportional changes to the peak dose.

7.9 OPEN REVIEW COMMENTS

In January 2020, a DOE review team evaluated the adequacy of this analysis to support a DOE Order 435.1 performance assessment. The review team acknowledged the iterative process that is being taken to evaluate closure of WMA A-AX. The review team made two recommendations to be considered for the next iteration of the uncertainty analysis.

The team recommended that additional uncertainty parameters be added to the model. The recommendation focused on the statement made in Appendix A Section A2.7.2 that it is expected that the model would be insensitive to saturated zone dispersivity. It was recommended that the model be revised to use the GoldSim plume function to evaluate uncertainty in the saturated zone longitudinal, transverse-horizontal, and transverse-vertical dispersivities.

In addition, the review team commented that triangular distributions for distribution coefficients that equate the minimum and most likely values may not be pessimistic. A triangular distribution that equates the minimum and most likely value will always sample values that are greater than the most likely value. A pessimistic evaluation would apply lower values for distribution coefficients, not higher values. Because a triangular distribution was used with a minimum and most likely value set to the same value, the sampled values are always higher than the most likely values. The review team recommended modifying the distribution type.

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APPENDIX A

DEVELOPMENT OF UNCERTAINTY PARAMETERS

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LIST OF TERMS, ACRONYMS, AND ABBREVIATIONS

DDI	distilled deionized (water)
DI	deionized (water)
HSU	hydrostratigraphic unit
LHS	Latin Hypercube Sampling
NCRP	National Council on Radiation Protection and Measurements
PA-TCT	Power Averaging-Tensorial Connectivity Tortuosity
PVC	polyvinyl chloride
RCRA	*Resource Conservation and Recovery Act of 1976*
SI	saturation index
SPFT	single-pass flow-through
STOMP	Subsurface Transport Over Multiple Phases
TIC	total inorganic carbon
WMA	Waste Management Area

A1.0 INTRODUCTION

Sensitivity and uncertainty analyses are required as part of the performance assessment. The guidance for completing the sensitivity and uncertainty analyses (DOE G 435.1-1, *Implementation Guide for Use with DOE M 435.1-1, Radioactive Waste Management Manual*) states that the dose rates have associated uncertainties, and a discussion of uncertainties should be included in expressing the outcomes of any performance assessment. The guidance further states that an estimate of the degree of uncertainty is needed for the analysis that includes the calculation of the maximum impact of the disposal facility beyond the 1,000-year compliance period.

Sensitivity analyses are complimentary to the uncertainty analysis and evaluate the changes from the base case that represent alternative conceptual models or alternative scenarios for the future evolution of the facility. In the current performance assessment, sensitivity analyses have been selected to represent the degradation of various key safety functions, as described in "A Hybrid Approach to the Use of Safety Functions with Features, Events, and Processes (FEPs) in Performance Assessment" (Kozak and Bergeron 2017.) These sensitivity analyses are document in RPP-CALC-63247, "WMA A-AX Performance Assessment Sensitivity Analysis".

NCRP Report 152, *Performance Assessment of Near-Surface Facilities for Disposal of Low-Level Radioactive Waste* notes that

> "methods of uncertainty and sensitivity analysis have been studied extensively, and a large body of scientific literature is devoted to each. However, that literature and the experience developed from it must be used with caution in the context of performance assessment, due to the unusual nature of this type of assessment and the significant amount of judgment that must be exercised. Results of uncertainty and sensitivity analyses of performance assessments need to be interpreted carefully, lest an erroneous and unwarranted implication of precision in calculations be imputed."

The National Council on Radiation Protection and Measurements (NCRP) emphasized that the goal of the uncertainty analysis is to support the regulatory decision, and that its nature and structure is therefore different than an uncertainty analysis focused solely on understanding uncertainties in model results.

A1.1 UNCERTAINTY ANALYSIS APPROACH

A1.1.1 General Approach

Uncertainties of importance in safety assessment may be due to stochastic variation or lack of knowledge ("On the Quantitative Definition of Risk" [Kaplan and Garrick 1981]). Stochastic variation refers to the variability attributed to a property of a system based on repeated measurements, and is referred to as aleatory uncertainty, or "Type A" (*Evaluating the Reliability of Predictions Made Using Environmental Transfer Models* [IAEA 1989]). Uncertainty due to

lack of knowledge is founded on an incomplete characterization, understanding or measurement of a system, and is referred to as epistemic uncertainty, or "Type B" (IAEA 1989). Epistemic uncertainties generally are the most important in safety assessments of waste disposal facilities (NCRP Report 152), because

- measurements made to support assessments tend to be limited,
- model parameters are often based on interpretations of data rather than direct measurement, and
- time scales and space scales of importance in safety assessment are not amenable to direct measurement.

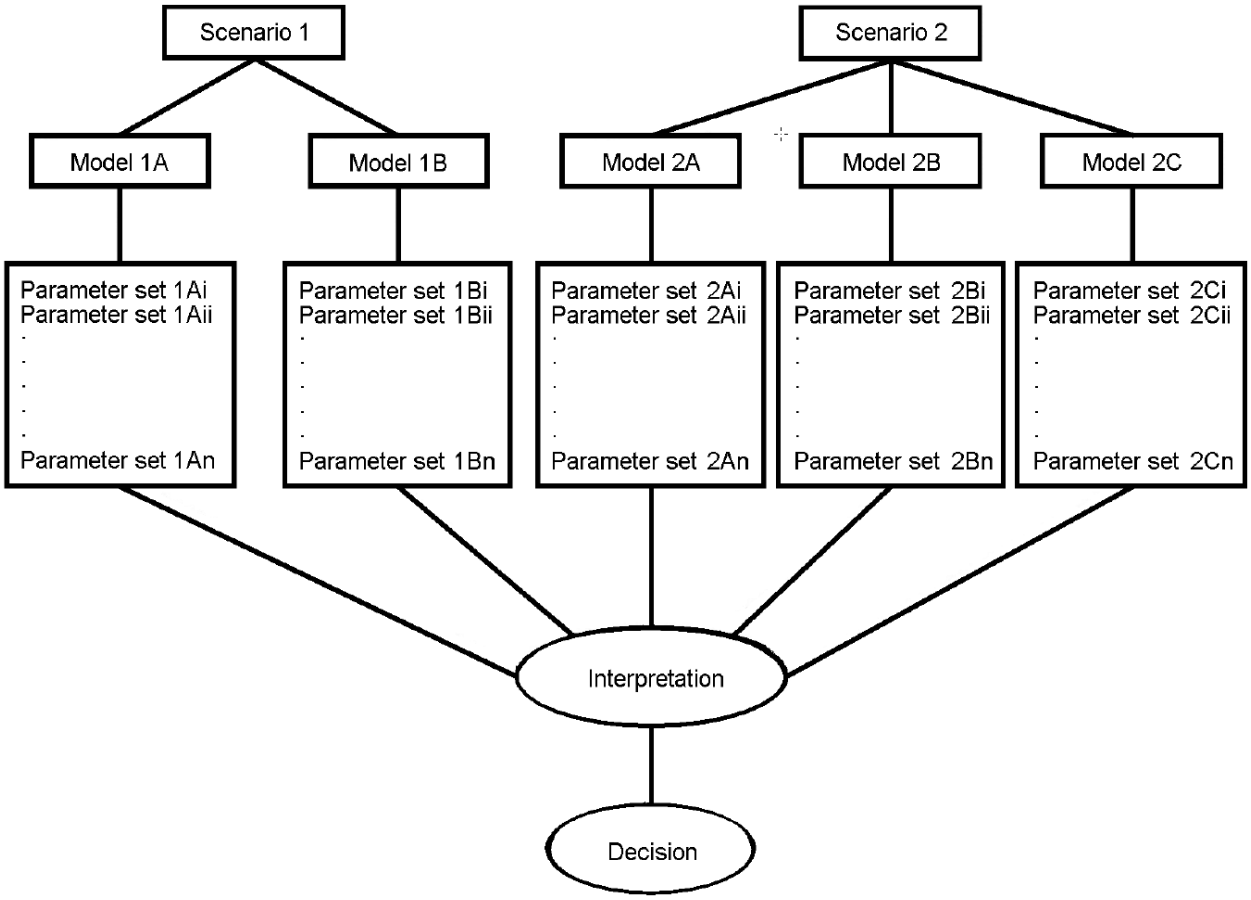
Further classification of uncertainties in safety assessment into uncertainties about models, uncertainties about the future, and uncertainties in model parameters is often used, even though such a classification is not fundamental (NCRP Report 152). The application of this classification allows the distinction between approaches to address the uncertainties as part of the safety assessment, using alternative scenarios and conceptual models, and addressing a range of parameters. A general structure of uncertainties represented in this way is shown in Figure A1-1.

It is crucial to recognize the unusual nature of safety assessments when considering uncertainty ("Decision Analysis for Low-Level Radioactive Waste Disposal Facilities" [Kozak 1994]; "Sensitivity, Uncertainty, and Importance Analyses" [Kozak 1997]). The uncertainty assessment needs to match the needs of the phase of the safety assessment to which it is applied. First, the magnitude of the projected dose needs to be known, and needs to be compared to the performance objective. Second, the credibility of that output needs to be established. Because of the limited amount of data to support performance assessments, projected doses will be uncertain. Consequently, the key issue is to identify the conditions for which uncertainty in assumptions or parameters can result in an altered decision. If the decision can be demonstrated to be insensitive to judgments about uncertainty in scenarios, conceptual models, and parameter values, the decision can be defended with confidence.

Consequently, the approach to be used for the performance assessment is to consider a range of credible scenarios and conceptual models and combinations of parameter values and determine if any credible combinations could result in a decision of non-compliance. These combinations will then be evaluated to show that there is reasonable assurance that they are inconsequential.

As noted by NCRP Report 152, both deterministic and probabilistic approaches can be appropriate for use in evaluating the uncertainties in a safety assessment, and each can be viewed as complementary to the other. These various approaches may be viewed as alternative approaches to assigning weighting factors to the alternative sets of scenario, model, and parameters shown in Figure A1-1. However, among the different uncertainty and sensitivity analysis approaches available, the Monte Carlo method has been most frequently used for performance assessments, and has been used for the current assessment.

Figure A1-1. General Structure of an Approach to Uncertainty Analysis for Safety Assessment.



Excerpted from NCRP Report 152, *Performance Assessment of Near-Surface Facilities for Disposal of Low-Level Radioactive Waste*.

In Monte Carlo analysis, discrete sets of input parameter values are selected at random from probability distribution functions; each set is run through the model, and a probability distribution function of model output is constructed. That distribution represents the uncertainty in model output associated with the uncertain input parameters. Among its main assets, this method is conceptually simple and able to cover the full range of parameter uncertainties.

The Monte Carlo approach involves the following steps ("Uncertainty and sensitivity analysis techniques for hydrologic modeling" [Mishra 2009]):

- Selecting model input parameters
- Assigning probability distributions to input parameters to quantify uncertainty
- Generating many sample sets (realizations) through sampling of probability distribution
- Propagating the uncertainty (via realizations) through the analysis
- Constructing an output distribution using either parametric or nonparametric approaches.

When carrying out Monte Carlo analyses, it is necessary to ensure that a sufficiently large set of input vectors has been sampled to produce stable estimates of the output distribution. Alternative approaches exist for identifying the parameter values that populate each vector. Of these approaches, the Latin Hypercube Sampling (LHS) approach has proved to be effective in producing stable estimates of the output distribution using fewer input realizations than, for instance, random sampling. In LHS, each input probability distribution is divided into equally likely strata or slices equal to the number of realizations. The strata are then "shuffled" into a random sequence, and a random value is picked from each stratum in turn. This approach ensures that the range of each of the input distributions is spanned with a relatively small number of realizations.

A1.1.2 Rationale for Assigning Probability Distributions

As noted above, uncertainties examined in performance assessments are dominated by epistemic uncertainties. For distributions representing epistemic uncertainties, Technical Report TR-02-11, *Assigning probability distributions to input parameters of performance assessment models* recommends choosing a probability distribution function by considering the principle of maximum entropy. In this approach, a distribution is chosen that preserves the maximum uncertainty about the data, similar to the well-known concept of thermodynamic entropy related to the degree of disorder or randomness. The principle of maximum entropy seeks to choose a probability distribution function that maximizes the informational entropy, subject to known constraints.

From a practical perspective, the use of the maximum entropy principle in assigning a distribution function implies the following considerations.

- If the only information on a parameter is its range of potential values, then all the samples are considered equally likely, and maximum entropy corresponds to a uniform distribution.

- If additional information is available, uncertainty is reduced, and a more refined type of distribution is suggested by maximum entropy. The appropriate shape of the distribution can be derived from the type of additional information about the input parameter using the entropy approach.

Based on these considerations, the maximum entropy principle implies that certain probability distribution functions are more appropriate for representing data with specific constraints, as summarized in Table A1-1. This approach has been used in this performance assessment for assigning distribution functions.

Several studies have tried to assess the impact of a chosen distribution function on the sensitivity analysis results. For instance, the results obtained by "The Effect of Distribution Choice for Uncertain Parameters in a Monte Carlo Analysis" (Hoffman 1996) can be used as a rule of

thumb for focusing the attention on parameter distributions that will have a relevant impact. Hoffman's conclusions are summarized in the following:

- As long as the uncertainty of a given parameter is small (coefficient of variation ≤30%), it makes very little difference which distribution is chosen
- As the coefficient of variation approaches and exceeds 30%, the use of distributions of log-transformed values is recommended
- The choice of distribution shape will be important if the analyst is interested in extreme values.

Table A1-1. Guidance for Selection of Probability Distribution Function Considering the Data Constraints.

Constraint	Distribution
Upper bound, lower bound	Uniform
Minimum, maximum, mode	Triangular
Mean, standard deviation	Normal
Range, mean, standard deviation	Beta
Mean occurrence rate	Poisson

Reference: Reliability-Based Design in Civil Engineering (Harr 1987).

A2.0 SELECTION OF PARAMETER UNCERTAINTY DISTRIBUTIONS

This section provides a description of each parameter evaluated in the uncertainty analysis for the Waste Management Area (WMA) A-AX performance assessment.

A2.1 UNCERTAINTY IN RECHARGE RATES

Recharge rates have been estimated from studies conducted at the Hanford Site over the last 30 years. Recharge rates are based on estimate of downward water flux below the evapotranspiration zone representing deep drainage. Recharge rates are available for natural and disturbed soils, for soils with and without vegetation, and for various plant communities. In addition, recharge has been estimated for surface covers with varying plant communities. These estimates are based on lysimeter records, tracer tests (chloride mass balance), and computer simulations to match field data. PNNL-16688, *Recharge Data Package for Hanford Single-Shell Tank Waste Management Areas* and PNNL-14702, *Vadose Zone Hydrogeology Data Package for Hanford Assessments* provide primary sources of information on recharge estimates for the

Hanford Site that are relevant to tank farms. There is limited information specific to WMA A-AX.

The modeling approach used to calculated flow velocities and moisture contents for the vadose zone takes account of the spatial and temporal changes in recharge (RPP-RPT-60101, *Model Package Report Flow and Contaminant Transport Numerical Model Used in WMA A-AX Performance Assessment and RCRA Closure Analysis*). Temporal changes occur in the analysis taking account of surface vegetative conditions during the pre-operational, disturbed soil conditions during the operational phase of Hanford operations. During the operational period, spatial variability in recharge occurred because WMA A-AX and surrounding areas have had varying vegetative cover and disturbed surface conditions. These conditions are followed by a transition to a post-closure configuration with a surface barrier at an assumed closure date in the future, followed in turn by an assumed date at which the surface barrier ceases to function, after which recharge rates are assumed to return to their pre-Hanford values. This modeling approach allows the model to establish the flow velocities and moisture content distributions that exist antecedent to each of the changes in the surface conditions at the site, and the response to the vadose zone flow in response to the changes in surface conditions.

The residual waste performance assessment is focused on the post-closure period. Experience with uncertainty analyses in the WMA C performance assessment (RPP-ENV-58782, *Performance Assessment of Waste Management Area C, Hanford Site, Washington*) and observations of the vadose zone flow and contaminant transport in the process model (RPP-RPT-60101) suggest that the following approximations may be adopted for the uncertainty analysis.

- The transport of contaminants under the WMA is not strongly influenced by flow outside area outside of the fence line. As a result of this observation, constant best-estimate values are used for those areas.

- Antecedent moisture conditions created by the operational period affect the transport for a relatively short period of time after closure, at a time when the surface barrier strongly limits the rate of contaminant transport. Therefore, constant best-estimate values are used for the pre-operational and operational periods.

- Therefore, the uncertainty analysis is limited to representing the uncertainty in recharge during the post-closure period. The post-closure period is subdivided into periods with the surface barrier intact, and with the surface barrier degraded. Uncertainty distributions for these time periods are as follows.

  <u>Post-Closure Period with Intact Surface Cover</u>: For the area covered by the intact surface barrier, the recharge rate is expected to decline to nearly zero, as the modified *Resource Conservation and Recovery Act of 1976* (RCRA)-compliant surface cover is designed to prevent or significantly limit recharge. The design criteria of such a barrier are identified in BHI-00007, *Prototype Hanford Surface Barrier: Design Basis Document* and DOE/RL-93-33, *Focused Feasibility Study of Engineered Barriers for Waste Management Units in the 200 Areas*, and include limiting recharge to 0.5 mm/yr. The

design life of surface cover as a recharge barrier is assumed to be 500 years (DOE/RL-93-33).

Extensive laboratory and modeling work, and limited field testing of surface barriers, have been performed with results summarized in PNNL-14744, *Recharge Data Package for the 2005 Integrated Disposal Facility Performance Assessment*. Lysimeter testing has been performed for different surface barrier concepts, including a Modified RCRA Subtitle C Barrier with silt-loam layers having depths between 1 and 2 m. Lysimeter data from the prototype Hanford barrier ("Quest for the Perfect Cap" [Wing and Gee 1994]) have also been collected and analyzed. Finally, modeling has been performed to address potential climate change impacts and no vegetation impacts on surface barrier performance.

The lysimeter drainage data that have been collected since 1989 suggest that the recharge rate beneath surface barriers having at least 1 m of silt loam is zero under ambient precipitation conditions. Most of these lysimeters did not contain an asphalt layer. Simulation results reported in PNNL-14744 investigated the sensitivity of the lysimeter data to climate change, silt-loam hydraulic properties, vegetation changes, erosion, and dune formation above the surface barrier. Results indicated that the performance of these surface barriers was robust in that the estimated recharge rates remained below 0.1 mm/yr. For the cases investigated, only in the case of dune formation and no vegetation on the surface barrier were the simulated recharge rates above 0.1 mm/yr. To account for such uncertainty (dune formation and no vegetation) within the design life of the barrier, an upper-bound recharge of 0.9 mm/yr is considered as suggested by PNNL-14744 for the post-barrier design life.

Based on the available information, uncertainty in recharge during post-closure period with intact surface is developed through selection of a triangular distribution, with a minimum value of 0.1 mm/yr, a maximum value of 0.9 mm/yr, and mode of 0.5 mm/yr.

<u>Post-Closure Period with Degraded Surface Cover</u>: In the post-closure period after 500 years, the recharge barrier capability of the surface cover is assumed to be degraded. This recharge rate is applicable to the entire simulated duration (except for the first 500 years after closure) and influences the contaminant transport of residual tank waste through the vadose zone. It is expected that once the surface cover is degraded, the recharge will be similar to the recharge during the pre-operational phase, since the surface will most likely be indistinguishable from the surrounding surface in terms of vegetative cover. PNNL-14744 suggests that the performance of the barrier is not expected to change after its design life. Conclusions in PNNL-14744 indicate that the possibility of the most likely natural failure mechanisms (i.e., bioturbation of the silt loam layer, wind erosion, and accretion of windblown sand) of these natural systems is quite low with an appropriate design. The emplaced silt-loam soils should continue to perform as long as they remain in place.

To propagate uncertainty in post-closure recharge rate following degraded surface cover, a triangular distribution is chosen, with a minimum value of 0.5 mm/yr, a mode value of

1.9 mm/yr, and a maximum value of 5.2 mm/yr. This uncertainty range is the same as that chosen for the pre-operational phase recharge rates.

The uncertainty in recharge rates selected for the various time periods are summarized in Table A2-1.

Table A2-1. Spatial and Temporal Uncertainty in Recharge Rates Considered for Waste Management Area A-AX Post-Closure Time Period.

Surface Condition	Triangular Distribution		
	Minimum	**Maximum**	**Most Likely**
Post-Closure Period with Intact Surface Cover (Years 2020 – 2520)			
Undisturbed (Natural Vegetation)	0.5	5.2	1.9
Waste Management Area Surface Barrier	0.1	0.9	0.5
Late Post-Closure Period with Degraded Surface Cover (Years > 2520)			
Undisturbed (Natural Vegetation)	0.5	5.2	1.9
Waste Management Area Surface Barrier	0.5	5.2	1.9

A2.2 UNCERTAINTY IN RESIDUAL INVENTORY ESTIMATES

Past performance assessments (e.g., RPP-ENV-58782) have represented uncertainties in residual waste inventory estimates associated with estimates errors in inventory measurements and possible errors in process knowledge. However, at the current preliminary state of retrieval of WMA A-AX, and in the absence of measured contaminant concentrations in retrieved samples, application of probability density functions to the inventory is not considered to be a useful approach to addressing inventory uncertainties for this preliminary performance assessment. Instead, alternative analysis cases have been included as sensitivity analyses. The sensitivity analyses are intended to evaluate the implications of differing levels of success in completing retrieval. In future revisions of this preliminary performance assessment for WMA A-AX, it may be useful to revisit this approach to evaluating inventory uncertainties, as additional information becomes available and as retrieval from the tanks commences.

A2.3 UNCERTAINTY IN SOURCE-TERM TRANSPORT PARAMETERS

Several parameters determine the release rate from the base of the tanks and ancillary equipment into the underlying vadose zone. Three general parameters are treated as uncertain in this analysis: K_d on cementitious materials, diffusion coefficient through cementitious barriers, and solubility of uranium.

A2.3.1 Sorption on Cementitious Barrier Materials

Sorption in the grouts and concretes in various features of the closed WMA have been represented by linear K_d sorption values. Data are lacking for the specific cementitious materials of interest in this assessment. As a consequence, literature sorption databases have been used to select sorption values.

Selections for sorption values (K_d) have been made based on review of past reports that are focused on developing internally-consistent cement sorption databases for cementitious near-field material (hardened cement paste) based on the composition of cement porewaters and stage of cement degradation. Results of the review are presented in Table A2-2; the following comments relate to the principles applied to identifying values from the literature.

- Conditions in the closed tank farm are expected to be moderately oxidizing, owing to the position of the waste in unsaturated conditions. Where data are available to differentiate between oxidizing and reducing conditions, K_d values under oxidizing conditions are preferentially selected, as it leads to lower K_d values relative to reducing conditions.

- Cementitious material (grout or concrete) may have different chemical compositions; contaminant uptake mechanisms and cement phases may differ. Due to lack of information, the differences in sorption between various types of cements and concrete are not explicitly included in the distribution range.

- The selected K_d values are based on assumption of $Ca(OH)_2$ saturated waters contacting the waste, and therefore represent the so-called stage II of the chemical degradation of cementitious material. In this stage, chemical composition of the alkali-depleted cement pore water is controlled by the solubility of portlandite. The impact on K_d values during evolution of chemical conditions from stage I (higher alkali content and pH) to stage II is expected to be minor and incorporated within the uncertainty range.

- The reviews of SKB R-05-75, *Assessment of uncertainty intervals for sorption coefficients, SFR-1 uppföljning av SAFE* and NIROND-TR 2008-23 E, *Review of sorption values for the cementitious near field of a near surface radioactive waste disposal facility, Project near surface disposal of category A waste at Dessel* are more recent, and represent critical reviews and independent data from NAGRA NTB 02-20, *Cementitious Near-Field Sorption Data Base for Performance Assessment of an ILW Repository in Opalinus Clay* and PSI Bericht Nr. 95-06, *Sorption Databases for the Cementitious Near-Field of a L/ILW Repository for Performance Assessment*. Where appropriate values are available from these more recent references, they are preferred to the older ones.

- When K_d values are absent from these references, a value of zero has been assumed for the analyte since chemical equivalences between similar analytes have not been performed to justify nonzero K_d values. As necessary, chemical equivalences suggested by SKB R-05-75 may be used to update K_d values in future iterations of the performance assessment modeling.

- When there was significant disagreement between literature sources, the lower (less sorptive) K_d value has been chosen. For example, K_d values under oxidizing conditions were selected over those measured under reducing conditions. Selecting lower K_d values is not always a conservative approach; a conservative treatment that makes one radionuclide more mobile in the environment may reduce the risk from its decay products. Caution has been taken to ensure that risk is not under-evaluated by selecting lower K_d values for decay product successors.

The K_d values were compared to values used in Savannah River F and H tank farm performance assessments [WSRC-STI-2007-00369, *Hydraulic and Physical Properties of Tank Grouts and Base Mat Surrogate Concrete for FTF Closure* and WSRC-STI-2007-00607, *Chemical Degradation Assessment of Cementitious Materials for the HLW Tank Closure Project (U)*]. The values used for WMA A-AX are generally consistent with or more conservative than comparable values used for the facility-specific grout used at Savannah River. When WMA A-AX values are more conservative, it has been for one of the following two reasons.

- The grout used at Savannah River produces reducing conditions. In the absence of a specific grout formulation for WMA A-AX, it has been assumed that oxidizing conditions will exist in the grout, which leads to lower (more conservative) K_d values for some radionuclides of interest.

- The disposal system at WMA A-AX is very robust with respect to meeting performance objectives. As a result, when data were ambiguous or insufficient in any way, it was more efficient to make a conservative assumption about K_d than to spend resources to resolve the value in greater detail. So, for instance, when data are lacking for a contaminant it is assigned a value of zero.

A2.3.2 Uncertainty in Diffusion Coefficient

The effective diffusion coefficient of mobile contaminants (such as ^{99}Tc) through the combined grout and concrete base mat is considered a key parameter that controls the diffusive flux from the source. Over the past decade, several experiments have been conducted to determine the effective diffusion coefficient through concrete for relatively mobile contaminants under unsaturated conditions. The results of various experiments are presented in PNNL-23841, *Radionuclide Migration through Sediment and Concrete: 16 Years of Investigations*. Of particular interest are the sediment-concrete half-cell experiments conducted in Year 2008 (for a period of 351 days) with ^{99}Tc and stable iodine.

Laboratory-scale concrete mixtures were prepared by omitting coarse aggregates and using 40 to 60 mesh size sand instead. The concrete mix prepared consisted of mainly Type I/II sulfate-resistant portland cement (27%), Class F fly ash (4%), sand (51%), and steel fiber (4%). The water-to-cement ratio was 0.5.

Table A2-2. K_d Values (mL/g) for Grout/Concrete Used for Waste Management Area A-AX Performance Assessment.

Element	Minimum	Best	Maximum	Reference
Ac	3.00E+04	1.00E+05	3.30E+05	NAGRA NTB 02-20
Al	0	0	0	No relevant information
Am	2.00E+02	1.00E+03	5.00E+03	SKB R-05-75
B	0	0	0	No relevant information
C	1.00E+01	2.00E+02	4.00E+03	SKB R-05-75
Cd	2.00E+00	4.00E+01	8.00E+02	SKB R-05-75
Cm	2.00E+02	1.00E+03	5.00E+03	SKB R-05-75
CN	0	0	0	No relevant information
Co	4.00E+00	4.00E+01	4.00E+02	SKB R-05-75
Cr	0	0	0	No relevant information
Cs	1.00E-01	1.00E+00	1.00E+01	SKB R-05-75
Eu	1.00E+03	5.00E+03	2.50E+04	SKB R-05-75
F	0	0	0	No relevant information
Fe	0	0	0	No relevant information
H	7.14E-02	1.00E-01	1.40E-01	NAGRA NTB 02-20
Hg	0	0	0	No relevant information
I	3.00E-01	3.00E+00	3.00E+01	SKB R-05-75
Mn	0	0	0	No relevant information
Nb	1.00E+02	5.00E+02	2.50E+04	SKB R-05-75
Ni	8.00E+00	4.00E+01	2.00E+02	SKB R-05-75
NO_2	0	0	0	No relevant information
NO_3	0	0	0	No relevant information
Np	7.14E+01	1.00E+02	1.40E+02	NAGRA NTB 02-20
Pa	7.14E+01	1.00E+02	1.40E+02	NAGRA NTB 02-20
Pb	3.60E+02	5.00E+02	7.10E+02	NAGRA NTB 02-20
Pu	7.14E+01	1.00E+02	1.40E+02	NAGRA NTB 02-20
Ra	5.00E+00	5.00E+01	5.00E+02	SKB R-05-75
Rn	0	0	0	No relevant information
Se	1.00E-01	6.00E+00	4.00E+02	SKB R-05-75
Sm	1.00E+03	5.00E+03	2.50E+04	SKB R-05-75
Sn	2.50E+01	5.00E+02	1.00E+04	SKB R-05-75
Sr	5.00E-01	1.00E+00	5.00E+01	SKB R-05-75
Tributyl phosphate	0	0	0	No relevant information
Tc	7.14E-01	1.00E+00	1.40E+00	NAGRA NTB 02-20
Th	1.00E+03	3.00E+04	1.00E+06	NIROND-TR 2008-23 E
U	1.43E+03	2.00E+03	2.80E+03	NAGRA NTB 02-20
Zr	3.03E+03	1.00E+04	3.30E+04	NAGRA NTB 02-20

References:

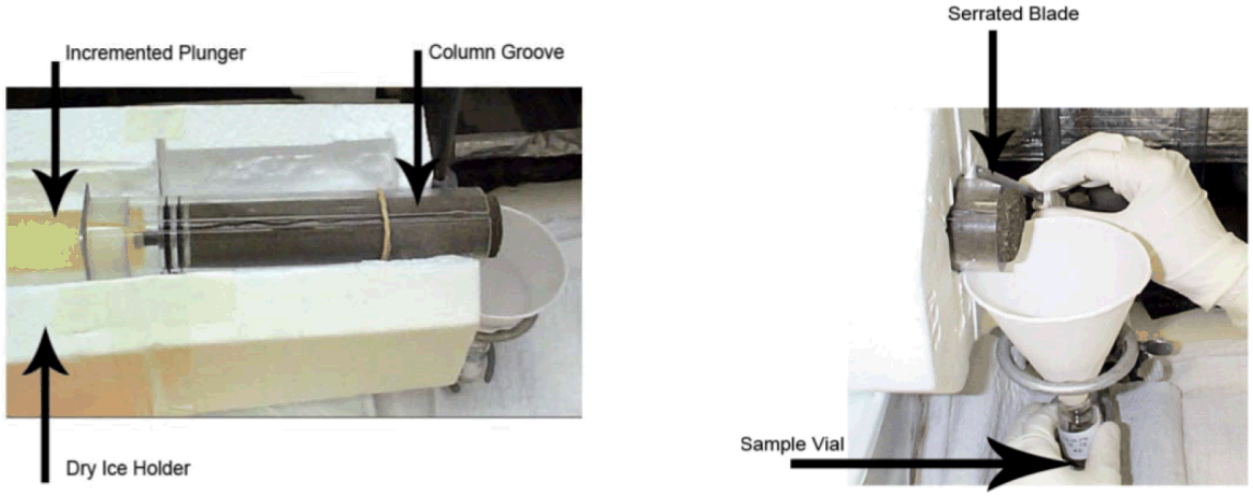
NAGRA NTB 02-20, *Cementitious Near-Field Sorption Data Base for Performance Assessment of an ILW Repository in Opalinus Clay*, Table 5.

NIROND-TR 2008-23 E, *Review of sorption values for the cementitious near field of a near surface radioactive waste disposal facility, Project near surface disposal of category A waste at Dessel*, Table 47.

SKB Rapport R-05-75, *Assessment of uncertainty intervals for sorption coefficients, SFR-1 uppföljning av SAFE*, Table 6-1.

The experiments were conducted using cylindrical cells made of Schedule 40 polyvinyl chloride (PVC) pipe (Figure A2-1). Caps were machined to fit into both ends of the PVC pipe and fitted with O-rings to minimize moisture loss during the test. For the sediment-concrete half-cells, the cell containing contaminant-spiked sediment was placed in contact with the non-spiked concrete monolith. The diffusion tests were run horizontally and undisturbed, with periodic rotation of the cell by 90 degrees. At the completion of the experiment, the concrete half-cells were sectioned parallel to the sediment-concrete interface. The concrete slices were then ground and two-to-one extracts (due to small sample size) by mass were performed on concrete fractions using the distilled deionized (DDI) water.

Figure A2-1. Set-Up of the Diffusive Half-Cell Experiment Contacting Contaminant-Spiked Sediment (or Concrete) Sample with the Non-Spiked Sediment (or Concrete) Sample.



The concentration profiles developed in the concrete were analyzed by fitting the analytical solution to Fick's second law, with the assumption of zero concentration downstream boundary condition, and deriving a bulk diffusion coefficient for the media. This bulk diffusion coefficient implicitly incorporates the effects of porosity and tortuosity due to diffusion that primarily occurs along the water films in the concrete. For the purpose of modeling mass transport along the water (liquid) phase the effective diffusion coefficient in the water phase is needed (instead of bulk diffusion coefficient), which can be derived by multiplying bulk diffusion coefficient with the moisture content. Since the moisture content of the base mat concrete and grout material is not known and would likely change with time due to slow but steady physical and chemical degradation, the effective diffusion coefficient is chosen conservatively to be the same as the measured bulk diffusion coefficient for the purpose of source-term modeling. In other words, the reduction due to multiplying with moisture content is not applied for calculating the diffusive flux. Note that the effective diffusion coefficient incorporates the effects of tortuosity resulting from transport along water films in the porous media.

Sediment-concrete diffusion experiments were initiated to investigate the effect of sediment moisture, concrete iron content, and concrete carbonation on the diffusivity of ^{99}Tc from sediment into concrete (PNNL-23841, Section 4.2.2). Sediment half-cell specimens were spiked

with ^{99}Tc (4.2×10^{-4} mg ^{99}Tc/g sediment) to achieve a measurable diffusion profile in the concrete part of the half-cell. Hanford fine sand was used for the sediment half-cell. In these experiments, iron content was varied in the concrete specimens from 0% to 12%, sediment moisture content was varied (4%, 7%, or 15%), and half of the concrete monoliths were carbonated prior to preparing the half-cells. The characteristics of the concrete half-cells are listed in Table A2-3. Half-cell sampling was conducted at 351 days. Figure A2-2 presents the concentration profile developed in the concrete.

The calculated effective diffusion coefficients of ^{99}Tc derived from the experimental results are presented in Figure A2-3 and tabulated in Table A2-3. They range from 6.6×10^{-9} cm^2/s to 1.6×10^{-7} cm^2/s (1.0×10^{-7} in.^{2}/s to 2.5×10^{-6} in.^{2}/s), with a median value of about 3×10^{-8} cm^2/s (4.7×10^{-7} in.^{2}/s). No particular measurable trend exists to indicate whether the effective diffusion coefficient varies with moisture content of the sediment. The highest ^{99}Tc diffusivities were predominantly observed in the non-carbonated concrete cores contacting spiked sediments. A clear effect from the addition of iron was not observed. In general, the increased carbonation reduced diffusion coefficients.

Similar experiments, as described above, were performed using stable iodine in 2008, where the sediment half-cell specimens were spiked with stable iodine at concentrations of ~7 mg of iodine per gram (246.9 oz/ton) of sediment (PNNL-23841, Section 4.1.2). Evaluation of the concentration profiles developed in the concrete half-cells were evaluated and the effective diffusion coefficient was determined for iodine, which ranged from 1.4×10^{-8} cm^2/s to 9.7×10^{-8} cm^2/s (2.17×10^{-7} in.^{2}/s to 1.50×10^{-6} in.^{2}/s) with a median value of 2.6×10^{-8} cm^2/s (4.03×10^{-7} in.^{2}/s). The non-carbonated samples exhibited a larger depth of diffusion compared to the carbonated samples, similar to the observations made for ^{99}Tc. The range of effective diffusion coefficient (and the median value) for iodine in concrete is very similar to that for ^{99}Tc.

Experiments were also performed to assess the effect of fractures in the concrete on diffusion of ^{99}Tc and iodine. For this purpose, the concrete monoliths were wrapped in shrink-wrap (to prevent the formation of rubble), and the end of the flathead screwdriver was placed directly in the center of the core and stuck once. Each fractured concrete monolith had a single midline fracture that penetrated the length of the core. A set of sediment to fractured concrete diffusion half-cell experiments were conducted, by varying the iron content using both carbonated and non-carbonated concrete but keeping the moisture content in the sediment half-cell constant at 4%. The sediment half-cell specimens were spiked with ^{99}Tc at a concentration of 3.24×10^{-4} mg per gram (0.011 oz/ton) of sediment. The derived effective diffusion coefficient ranged from 1.9×10^{-9} cm^2/s to 2.5×10^{-8} cm^2/s (2.94×10^{-8} in.^{2}/s to 3.88×10^{-7} in.^{2}/s). Similar experiments conducted using stable iodine (spiked at 7 mg per gram [246.9 oz/ton] of sediment) resulted in effective diffusion coefficient that ranged from 4.7×10^{-9} cm^2/s to 8.4×10^{-8} cm^2/s (7.29×10^{-8} in.^{2}/s to 1.30×10^{-6} in.^{2}/s). These ranges are similar to the ranges calculated for diffusion in the unfractured concrete monolith.

Table A2-3. Characteristics of Concrete Specimens Used in Sediment-Concrete Half-Cell Experiments Along with Derived Bulk Diffusion Coefficient of Technetium-99 for the Concrete.*

Core ID	Length (cm)	Diameter (cm)	Surface Area (cm^2)	Volume (cm^3)	Weight (g)	Density (g/cm^3)	Iron (wt%)	Carbonated	Initial Sediment Moisture Content (%)	Technetium-99 Diffusivity (cm^2/s)
C-08-3-0-325	4.09	4.33	84.97	60.1	131.44	2.19	0	No	4	7.08E-08
C-08-3-0-329	4.32	4.33	88.13	63.53	139.5	2.2	0	No	7	6.55E-08
C-08-3-0-330	3.85	4.33	81.77	56.65	123.5	2.18	0	No	15	3.51E-08
C-08-3-0-332	4.33	4.32	88.09	63.48	139.65	2.2	0	Yes	4	2.23E-08
C-08-3-0-333	4.35	4.33	88.57	64	140.79	2.2	0	Yes	7	2.25E-08
C-08-3-0-334	4.07	4.32	84.56	59.67	130.55	2.19	0	Yes	15	1.22E-08
C-08-3-4-350	3.84	4.32	81.43	56.28	127.25	2.26	4	No	4	3.21E-08
C-08-3-4-351	4	4.33	83.92	58.96	132.78	2.25	4	No	7	1.57E-07
C-08-3-4-353	4.01	4.33	83.99	59.04	133.38	2.26	4	No	15	3.09E-08
C-08-3-4-357	3.9	4.32	82.19	57.11	128.77	2.25	4	Yes	4	3.09E-08
C-08-3-4-359	3.83	4.32	81.25	56.09	126.5	2.26	4	Yes	7	1.07E-08
C-08-3-4-360	4.11	4.33	85.47	60.64	136.11	2.24	4	Yes	15	3.26E-08
C-08-3-8-401	4.07	4.32	84.4	59.5	135.91	2.28	8	No	4	7.76E-09
C-08-3-8-402	3.81	4.32	81.02	55.84	127.31	2.28	8	No	7	2.85E-08
C-08-3-8-403	4	4.33	83.87	58.91	133.35	2.26	8	No	15	1.62E-08
C-08-3-8-404	4.05	4.33	84.61	59.71	133.69	2.24	8	Yes	4	5.34E-08
C-08-3-8-405	3.86	4.33	81.77	56.65	126.96	2.24	8	Yes	7	9.25E-09
C-08-3-8-406	3.94	4.33	83.08	58.05	130.61	2.25	8	Yes	15	6.61E-09
C-08-3-12-425	4.33	4.27	87.54	62.88	143.44	2.28	12	No	4	1.07E-07
C-08-3-12-426	4.33	4.33	88.35	63.76	145.77	2.29	12	No	7	1.31E-08
C-08-3-12-427	4.33	4.22	86.94	62.23	141.71	2.28	12	No	15	8.21E-08
C-08-3-12-432	4.02	4.32	83.83	58.88	134.09	2.28	12	Yes	4	4.6E-08
C-08-3-12-433	4.15	4.33	85.81	61.01	139.8	2.29	12	Yes	7	6.95E-09
C-08-3-12-435	3.88	4.33	82.22	57.12	130.04	2.28	12	Yes	15	7.09E-09

*Note: For the purpose of source-term calculations, the bulk diffusion coefficient is considered to be the same as effective diffusion coefficient.

Figure A2-2. Technetium-99 Concentration Profiles in Concrete from Sediment-Concrete Half-Cell Experiments Conducted on (A) 4% Sediment Moisture, Carbonated Monoliths, (B) 4% Sediment Moisture, Non-Carbonated Monoliths, (C) 7% Sediment Moisture, Carbonated Monoliths, (D) 7% Sediment Moisture, Non-Carbonated Monoliths, (E) 15% Sediment Moisture, Carbonated Monoliths, and (F) 15% Sediment Moisture, Non-Carbonated Monoliths.

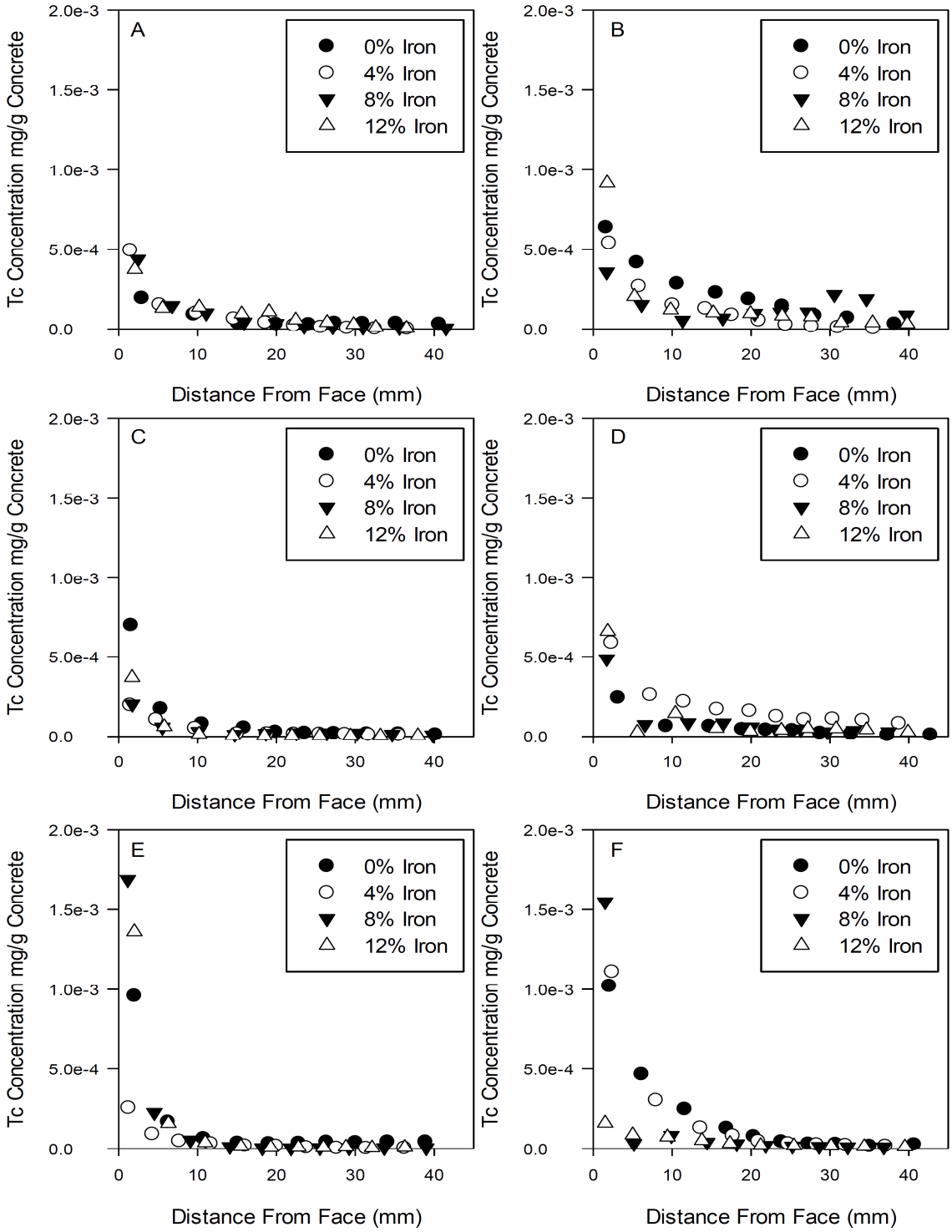
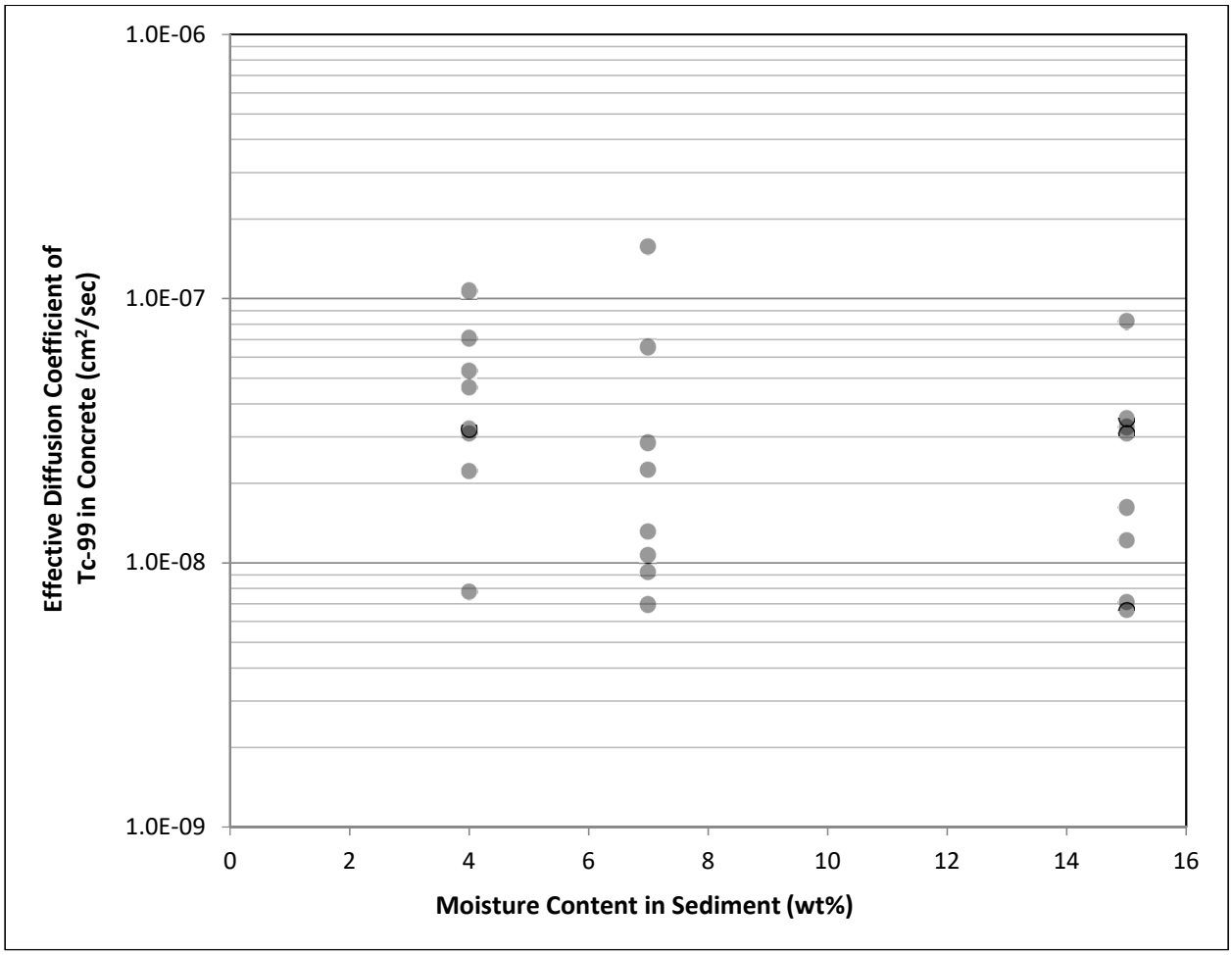


Figure A2-3. Effective Diffusion Coefficient of Technetium-99 in Concrete Based on Experiments Conducted Using Sediment-Concrete Half-Cells.



Reference: PNNL-23841, *Radionuclide Migration through Sediment and Concrete: 16 Years of Investigations*.

For the purpose of deterministic base case analysis, the experimental median value of 3×10^{-8} cm^2/s (4.65×10^{-7} in.^{2}/s) has been chosen. This value is applied to all species diffusing through the concrete. Based on the range presented in Figure A2-3, an uncertainty range with a minimum and maximum value of 6×10^{-9} cm^2/s and 2×10^{-7} cm^2/s (9.30×10^{-8} in.^{2}/s and 3.10×10^{-6} in.^{2}/s), respectively, has been adopted. Therefore, the probability density function for effective diffusion coefficient through the base mat has been assigned a log-uniform distribution with a minimum and maximum value of 6×10^{-9} cm^2/s and 2×10^{-7} cm^2/s, respectively, and a median value of 3.5×10^{-8} cm^2/s. This median value is close to the best-estimate value of 3×10^{-8} cm^2/s.

A2.3.3 Solubility Limit for Uranium

Data are not yet available on retrieved samples from WMA A-AX residual wastes. In this section, an assumption has been made that testing and experiments conducted on wastes from

WMA C are representative for WMA A-AX. The appropriateness of this assumption should be revisited once data are collected from WMA A-AX wastes.

Laboratory leaching tests have been conducted on residual waste samples from various tanks from WMA C. "Single-pass flow-through test elucidation of weathering behavior and evaluation of contaminant release models for Hanford tank residual radioactive waste" (Cantrell et al. 2013) provided the analysis of residual waste following leaching with three different leachates—namely, deionized (DI) water, $CaCO_3$ saturated solution, and 0.005 M $Ca(OH)_2$ solution. These three leachates represent a range of possible water types contacting the residual waste. The $CaCO_3$ saturated solution was used to simulate a leachate produced by aged carbonate cement or a typical Hanford vadose zone pore water, 0.005 M $Ca(OH)_2$ solution was used to represent the likely influence of interaction of infiltrating vadose zone pore water with portlandite [$Ca(OH)_2$] in the grouted tanks, and the DI water was used as a baseline for the leach tests to evaluate the influence of waters that have not been altered by reactions with the $Ca(OH)_2$ and $CaCO_3$ leachates.

The general trends in uranium leachate concentrations for the 241-C-103, 241-C-202, and 241-C-203 tank residual wastes are very similar (RPP-ENV-58782). The leached uranium concentration using DI water and $CaCO_3$ saturated solution are significantly higher than those in the 0.005 M $Ca(OH)_2$ leachates. This is attributed to forming calcium-rich precipitates (calcium phosphate and calcite) on the surfaces of the waste particles when using $Ca(OH)_2$ leachate, inhibiting dissolution of the underlying uranium phases in the waste. Since the tanks are planned to be grouted prior to closure, the primary leachate is expected to be $Ca(OH)_2$ saturated solution ("Hanford tank residual waste – Contaminant source terms and release models" [Deutsch et al. 2011]), which is likely to reduce the leaching of uranium.

To investigate this leaching behavior, thermodynamic equilibrium modeling was conducted. The saturation indices (SIs) calculated for the tank 241-C-202 single-pass flow-through (SPFT) effluents for the three leachates indicated that DI water and $CaCO_3$ saturated leachate give similar SI results, while the $Ca(OH)_2$ leachate SI results are quite different. Results from DI water and $CaCO_3$ saturated leachates indicate that $NaUO_2PO_4.xH_2O$ is near equilibrium while calcium-containing phases (such as calcite and hydroxylapatite) were all undersaturated. The SI results for the $Ca(OH)_2$ leachates indicate all uranium-bearing phases to be highly undersaturated but are near-saturated or oversaturated with respect to calcium-containing phases. Calcite was near saturation, while hydroxylapatite and flourapatite were consistently highly oversaturated.

These results are consistent with the observed leaching behavior of uranium. It is hypothesized that precipitation of calcium-rich phases resulted in coatings on the waste particles that could have temporarily inhibited dissolution and attainment of equilibrium for any uranium phase in contact with $Ca(OH)_2$ leachate solutions.

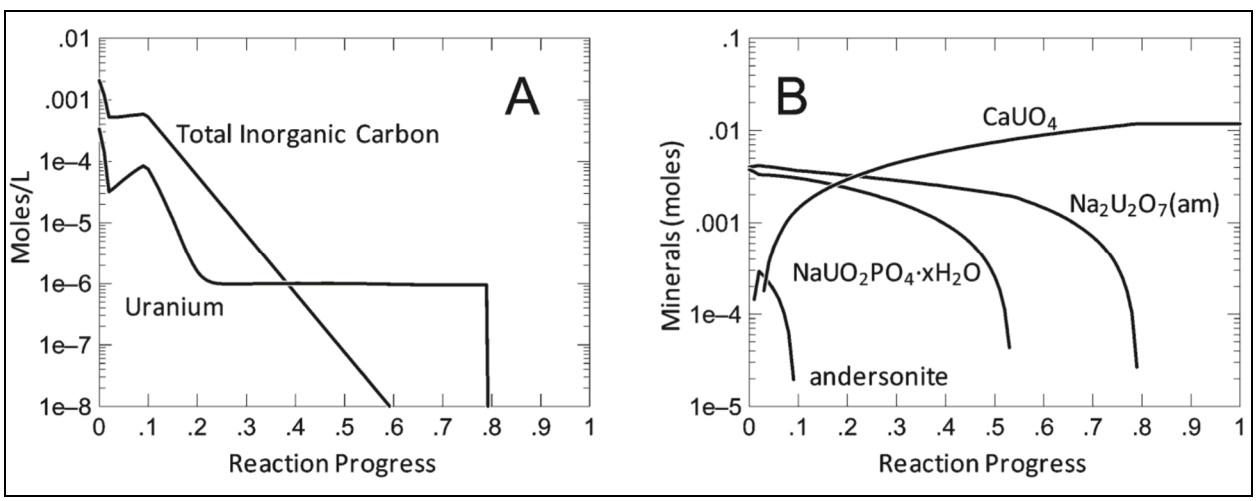
These results indicate that as long as the infiltrating water though the tank passes through the infill grout material, it will be conditioned to be similar to a dilute $Ca(OH)_2$ leachate solution and the uranium dissolution will remain inhibited (Cantrell et al. 2013). At some distant time in the future when the tank is assumed to be sufficiently degraded such that large open fractures develop that do not allow appreciable residence time for infiltrating waters to contact and

equilibrate with the grout material, the leachate would be similar to the $CaCO_3$ saturated water, and at that time the uranium concentrations may increase when the residual waste is contacted.

Reaction-path modeling was undertaken in "Thermodynamic Model for Uranium Release from Hanford Site Tank Residual Waste" (Cantrell et al. 2011) to evaluate the uranium release under the $Ca(OH)_2$ and $CaCO_3$ saturated waters by applying an infiltration rate of 1 mm/yr (0.039 in./yr) through the tank material over 10,000 years. The steel of the tank itself was assumed to have no impact on the hydrology or system chemistry, and the waste was assumed to be uniformly distributed at the bottom of the tank. The results of this reaction-path modeling are summarized below.

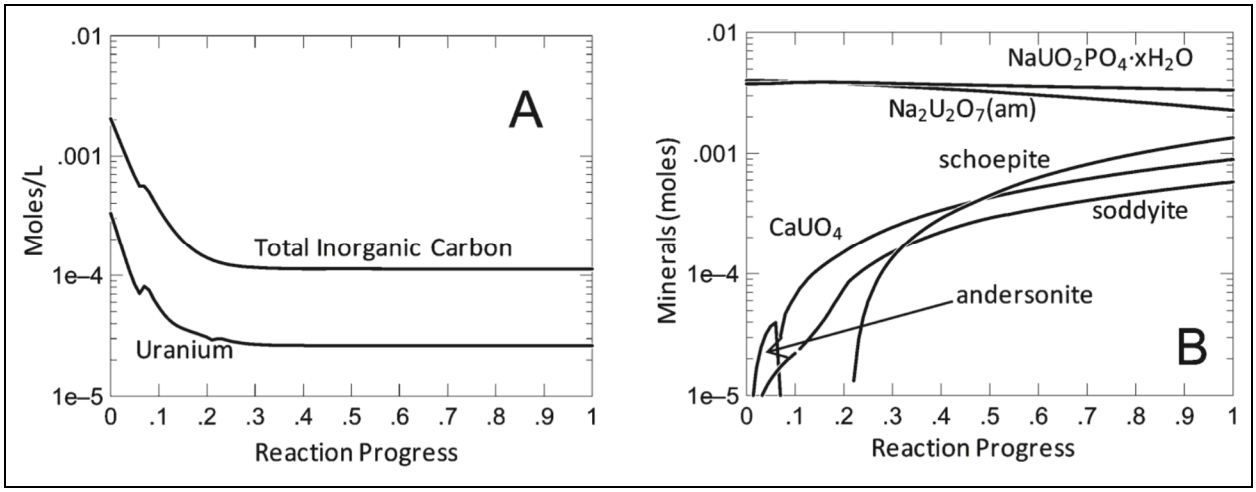
For $Ca(OH)_2$ saturated water, the tank was assumed to be filled with cementitious material (i.e., concrete or grout), and the composition of the simulated pore water was assumed to be 0.015 M $Ca(OH)_2$ and 1×10^{-5} M SI. The results of the reaction progress in terms of the uranium and total inorganic carbon (TIC) concentrations and the paragenetic sequence of uranium phases over the course of 10,000 years are shown in Figure A2-4. Initially, high uranium concentrations occur in solution (~3×10^{-4} M) because of high carbonate complexation of uranium, but decline rapidly and rebound somewhat as a small amount of andersonite [$Na_2CaUO_2(CO_3)_3.6H_2O$] first precipitates and then dissolves. As the reaction progress continues, $NaUO_2PO_4.xH_2O$ dissolves preferentially to $Na_2U_2O_7$(am). As carbonate continues to leach from the waste, uranium concentrations continue to decline until a plateau is reached at approximately 1×10^{-6} M. This occurs at the approximate point where $CaUO_4$ becomes the dominant phase. A dramatic reduction in uranium concentrations occurs when $Na_2UO_2O_7$ (am) dissolves completely, leaving $CaUO_4$ as the only phase to control uranium release concentrations. A reaction progress of 1.0 is equivalent to 1 mm/yr (0.039 in./yr) of flow for 10,000 years, and therefore represents 10,000 mm (394 in.) of flow.

Figure A2-4. Uranium and Total Inorganic Carbon Concentrations (A) and the Paragenetic Sequence of Uranium Phases Present in the Waste (B) as a Function of Reaction Progress for the $Ca(OH)_2$ Saturated Water Scenario. A reaction progress of 1 is equivalent to 10,000 years of infiltration at 1 mm/yr.



A similar reaction progress modeling calculation for the $CaCO_3$ saturated waters is shown in Figure A2-5. Initial high uranium concentrations in solution (~3 × 10^{-4} M) occur because of high carbonate complexation of uranium due to soluble Na_2CO_3 or cejkaite [$Na_4(UO_2)(CO_3)_3$]. As very soluble carbonate phases dissolve, the uranium concentration of about 2.6 × 10^{-5} M is maintained primarily by dissolution of $NaUO_2PO_4.xH_2O$ and $Na_2U_2O_7$(am), although schoepite ($UO_3 \cdot 2H_2O$) also becomes important.

Figure A2-5. Uranium and Total Inorganic Carbon Concentrations (A) and the Paragenetic Sequence of Uranium Phases Present in the Waste (B) as a Function of Reaction Progress for the $CaCO_3$ Saturated Water Scenario. A reaction progress of 1 is equivalent to 10,000 years of infiltration at 1 mm/yr.



Over the course of these simulations, 2% of the uranium in the waste is calculated to be dissolved in the $Ca(OH)_2$ saturated water, compared to 6.4% for the $CaCO_3$ saturated water. This is attributed to the formation of relatively insoluble $CaUO_4$ phase under high calcium and high pH conditions.

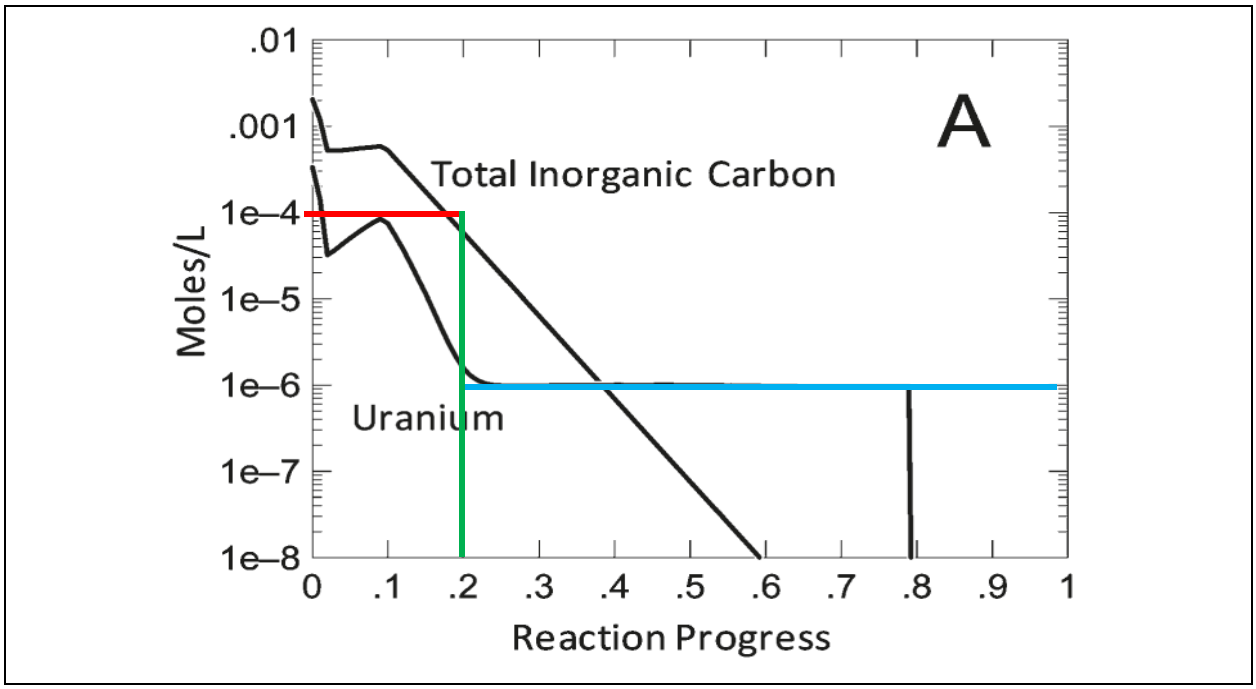
The results of the reaction progress modeling are used to impose solubility limits for uranium. As a conservative calculation, it is assumed that the infill grout is not a barrier to flow through the tank, and the recharge rates imposed on the backfill material (0.5 mm/yr [0.019 in./yr] for the first 500 years and 3.5 mm/yr [0.138 in./yr] afterwards) are also the flow rates through the tanks, even though the rates are likely to be far lower due to lower permeability. Given these flow rates, it is calculated that in the 1,000-year post-closure compliance time period, a total of 2,000 mm (78.7 in.) of water would flow (0.5 mm/yr [0.019 in./yr] × 500 years + 3.5 mm/yr [0.138 in./yr] × 500 years). This is equivalent to a reaction progress of 0.2 presented in Figure A2-4 and Figure A2-5. Using this information, the following solubility controls are imposed on the uranium concentrations for the base case, as shown in Figure A2-6.

- Apply solubility limit of 1 × 10^{-4} M for 1,000 years (equivalent to reaction progress of 0.2) based on the assumption that amorphous uranium mineral phases such as $Na_2U_2O_7$(am) control the solubility.

- After 1,000 years, apply the solubility limit of 1×10^{-6} M, assuming $CaUO_4$ as the solubility-controlling mineral phase under $Ca(OH)_2$ saturated conditions (infill grout saturated and intact-tank conditions).

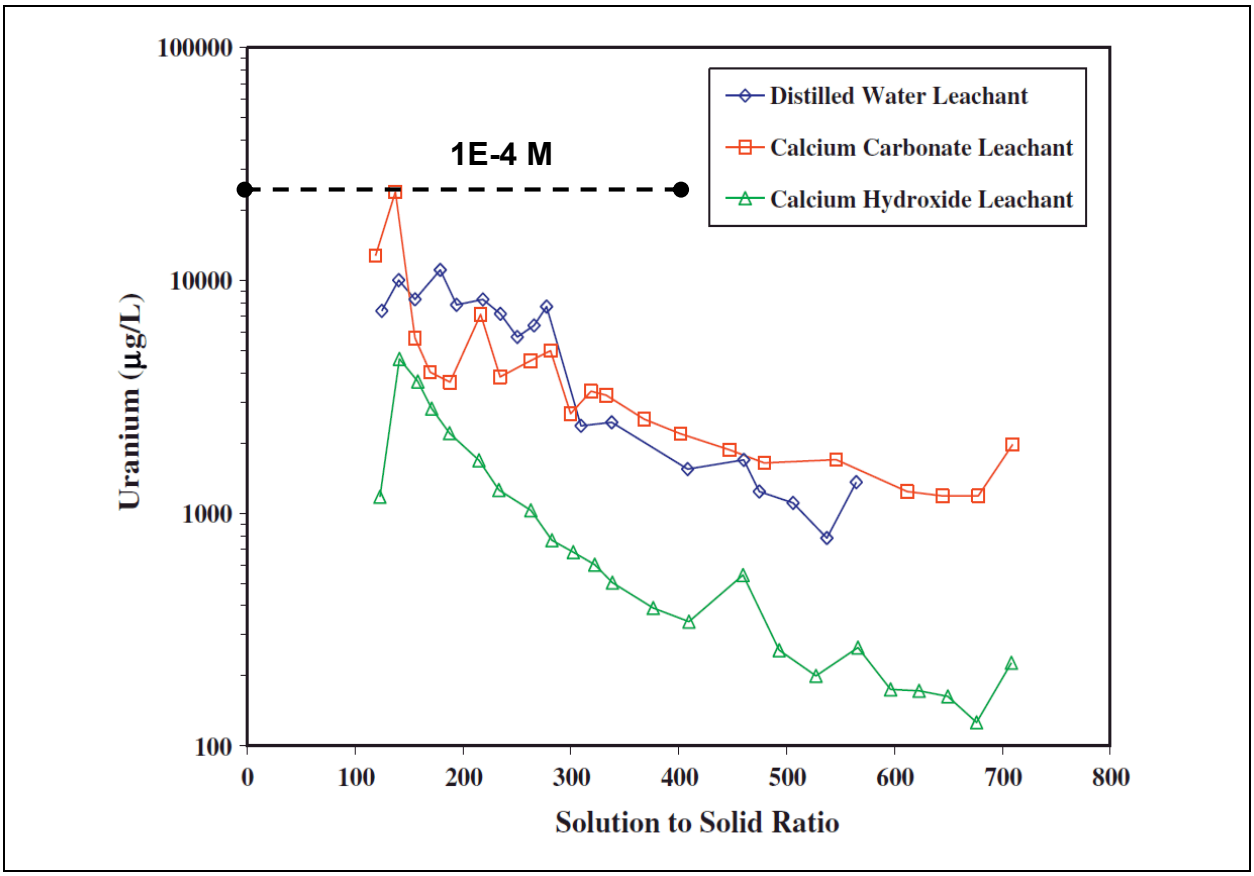
- For sensitivity analyses in which the tank is assumed to be degraded, it is assumed that flow rates are fast enough not to equilibrate with the infill grout material. It is therefore assumed that the water is $CaCO_3$ saturated (vadose zone water). A solubility limit of 2×10^{-5} M has been applied, based on the long-term uranium concentrations shown in Figure A2-5, assuming minimal influence of $Ca(OH)_2$ water.

Figure A2-6. Uranium Solubility Model Implemented with Solubility Limits Varying with Time. Reaction progress of 0.2 is equivalent to 1,000 years of flow under base case recharge conditions through the backfill material.



The reaction progress modeling calculations were performed under relatively static conditions. SPFT tests can be considered as analogous to column flow-through experiments. These are conducted under low flow conditions (~0.1 mL/hr [0.06 in.^{3}/hr]) for a period of about six months (at the sediment mass-to-solution ratio of 0.5 g [0.02 oz] to 0.06 L [3.66 in.^{3}]) with no stirring of the waste form in the solution. Even under these conditions, the application of the initial high solubility limit of 1×10^{-4} M is conservative for the 1,000-year time period. The SPFT test conducted on tank 241-C-202 residuals (Figure A2-7) indicates that peak uranium concentrations for the $CaCO_3$ saturated water reached the solubility limit 1×10^{-4} M for a short duration at an early time, but later dropped to much lower numbers, and therefore represents a likely bounding uranium solubility value under all conditions at WMA A-AX. This solubility limit is imposed for pipeline releases as well, where the releases are likely to be advectively dominated. This assumption is justified by the same logic about flow rates presented above.

Figure A2-7. Comparison of Initially Imposed Uranium Solubility Limit of 1 × 10^{-4} M to the Observed Concentrations during the Single-Pass Flow-Through Conducted on 241-C-202 Tank Residual.



The solubility of uranium is considered to be uncertain in the analysis. It is assumed that the uncertainty can be represented by a factor of two uncertainty multiplier to the solubility. This is implemented by assigning a log-uniform distribution varying from 0.5 to 2 to determine the bounds of the distribution. The mean solubility is assumed to change from 10^{-4} M to 10^{-6} M at 1,000 years. Therefore, the applied distributions are a log-uniform distribution between 5 × 10^{-5} and 2 × 10^{-4} M prior to 1,000 years and 5 × 10^{-7} and 2 × 10^{-6} M after 1,000 years. This distribution provides a median value of 1 (and mean is about 1.1); therefore, the mean/median sampled multiplier will retain the deterministic case solubility value.

A2.4 UNCERTAINTIES IN VADOSE ZONE FLOW FIELD

Vadose zone flow fields of interest for input to the GoldSim©[1] system model are represented by the Darcy velocity and moisture content. The flow fields have been abstracted from the

[1] GoldSim© simulation software is copyrighted by GoldSim Technology Group LLC of Issaquah, Washington (see http://www.goldsim.com).

three-dimensional Subsurface Transport Over Multiple Phases (STOMP)©[2] analyses (RPP-RPT-60101; RPP-CALC-63164, *WMA A-AX Performance Assessment Contaminant Fate and Transport Process Model to Evaluate Impacts to Groundwater*) to provide input to a one-dimensional approximation to the full three-dimensional flow field (RPP-RPT-60885, *Model Package Report System Model for the WMA A-AX Performance Assessment*; RPP-CALC-62538, *WMA A-AX Performance Assessment Groundwater Pathway Dose Calculation*). Uncertainties in the flow field for the GoldSim© model may be considered to be influenced by two interrelated and coupled sources:

- Uncertainty in the appropriate upscaled soil properties, as represented by the Power Averaging-Tensorial Connectivity Tortuosity (PA-TCT) model ("Simulating field-scale moisture flow using a combined power-averaging and tensorial connectivity-tortuosity approach" [Zhang and Khaleel 2010]) relating moisture content, pressure head, and unsaturated conductivity, and

- Uncertainty in the recharge rates (Section A2.1) and how moisture-dependent anisotropy influences the redistribution of recharge in the vadose zone.

Upscaling is the process of defining effective large-scale properties for the numerical model based on small, core-scale measurements ("Upscaled flow and transport properties for heterogeneous unsaturated media" [Khaleel et al. 2002]). In essence, upscaling identifies effective average properties appropriate for representing the mean flow behavior associated with the aleatory uncertainty in small-scale measurements.

Using the combined PA-TCT model, Zhang and Khaleel (2010) estimated the three-dimensional effective unsaturated hydraulic conductivity tensor for the Sisson and Lu field injection site near WMA A-AX in 200 East Area. Details of the Sisson and Lu site, field injections and the spatio-temporal distribution of observed moisture plume are described elsewhere ("Stochastic Analysis of Moisture Plume Dynamics of a Field Injection Experiment" [Ye et al. 2005]; Zhang and Khaleel 2010). Overall, the PA-TCT-based numerical results using low anisotropy compared well with the observed plume behavior at the Sisson and Lu site (Zhang and Khaleel 2010). This PA-TCT model is used in the WMA A-AX STOMP© process model to upscale the vadose zone hydraulic properties. Since this model is the conceptual representation of the vadose zone framework and the model has been compared with field observations at a nearby site, the hydraulic properties associated with this model represent the conceptual model of the vadose zone at WMA A-AX.

The uncertainty in the upscaled parameters has not been included in the uncertainty assessment; fixed parameter values are held at their upscaled values for the uncertainty analysis. A revised approach to address this uncertainty may be included in a future revision of the performance assessment as more information becomes available.

Although uncertainty in the upscaled parameters is not directly addressed in this performance assessment, uncertainty in vadose zone flow is considered. The uncertainty in the vadose zone flow field is accounted by correlating the moisture content and flow rate to the sampled recharge

[2] Subsurface Transport Over Multiple Phases (STOMP)© is copyrighted by Battelle Memorial Institute, 1996.

rates for an intact and degraded surface barrier. This uncertainty can be expressed as the relationship between the recharge rate and the associated abstracted vertical Darcy flow rate and moisture content in the GoldSim© vadose zone column.

At long times when the flow rate is at steady state, and far from any subsurface obstruction, a simple mass balance would suggest that the Darcy flow rate in the vadose zone should equal the recharge rate. However, the presence of the tanks in the subsurface causes a diversion of flow, such that the representative flow rate below the tanks abstracted for the GoldSim© model is slightly different than the recharge rate. Furthermore, the amount of diversion that occurs is dependent on the anisotropy, which itself is dependent on the moisture content. The result is that at higher recharge rates (higher moisture content), the Darcy flow rate under the tanks is somewhat higher than the recharge rate, while at low recharge rates it is somewhat lower. As discussed in RPP-ENV-58782, Appendix B, these effects have been observed to follow a linear relationship between both the vertical Darcy flow rate and the moisture content used in the GoldSim© model and the recharge rate when hydraulic properties remain unchanged. This linear relationship was developed as follows.

- Vertical Darcy flux velocity volumetric moisture content values were abstracted from STOMP© model nodes that correspond to the GoldSim© one-dimensional discretization. This was done for Calendar Year 2300 (to represent early the post-closure time period from Calendar Year 2020 to 2520 while the surface cover is intact) and at Calendar Year 5050 (to represent the late post-closure period beyond Calendar Year 2520 following surface barrier degradation).

- The extracted vertical Darcy velocity and volumetric moisture content were normalized by dividing by the values obtained from the base case recharge flow field.

- The normalization factors were evaluated by linear regression against recharge rate.

- These normalization factors are then multiplied by the base case Darcy velocity and moisture content for any value of recharge rate to produce the corresponding vadose zone flow rate and moisture content in the representative GoldSim© column.

The result is an equation for the effective Darcy velocity and moisture content for any sampled value of recharge rate. In the Monte Carlo analysis, for each realization of recharge rate, the regression equations produce the appropriate corresponding vertical Darcy flow rate and moisture content.

The regression analyses for the early period in the analysis, when the surface barrier is intact, are presented in Figure A2-8 and Figure A2-9. The regression analyses for the later period in the analysis, when the surface barrier is failed, are shown in Figure A2-10 and Figure A2-11.

Figure A2-8. Regression Equation for Ratio of Darcy Velocity to the Base Case Darcy Velocity as a Function of Recharge Rate: Intact Surface Barrier.

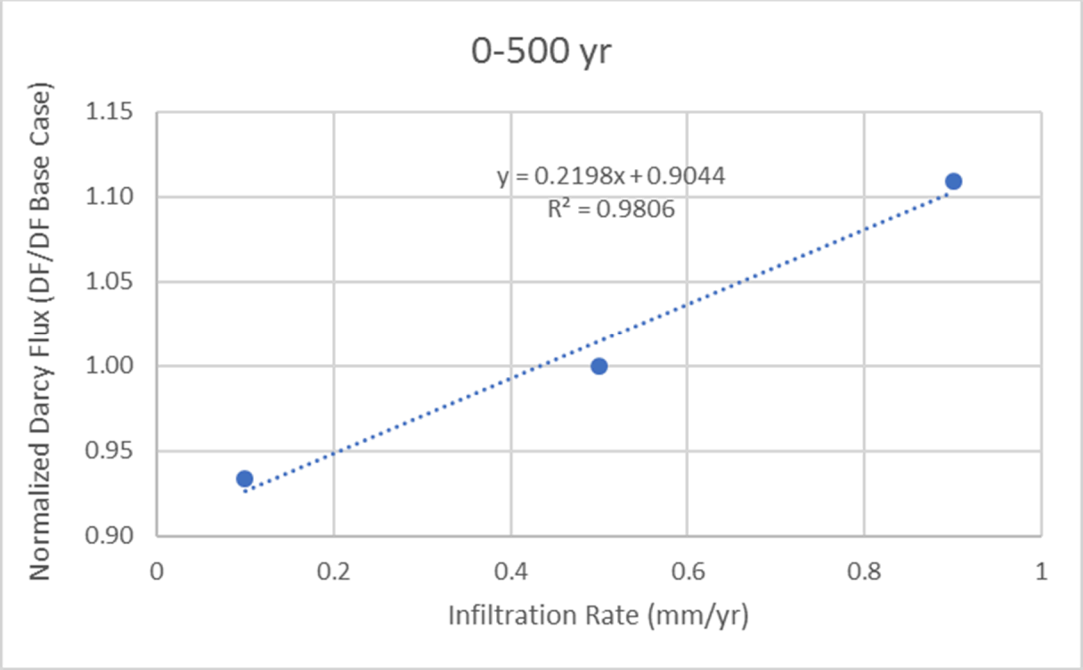


Figure A2-9. Regression Equation for Ratio of Moisture Content to the Base Case Moisture Content as a Function of Recharge Rate: Intact Surface Barrier.

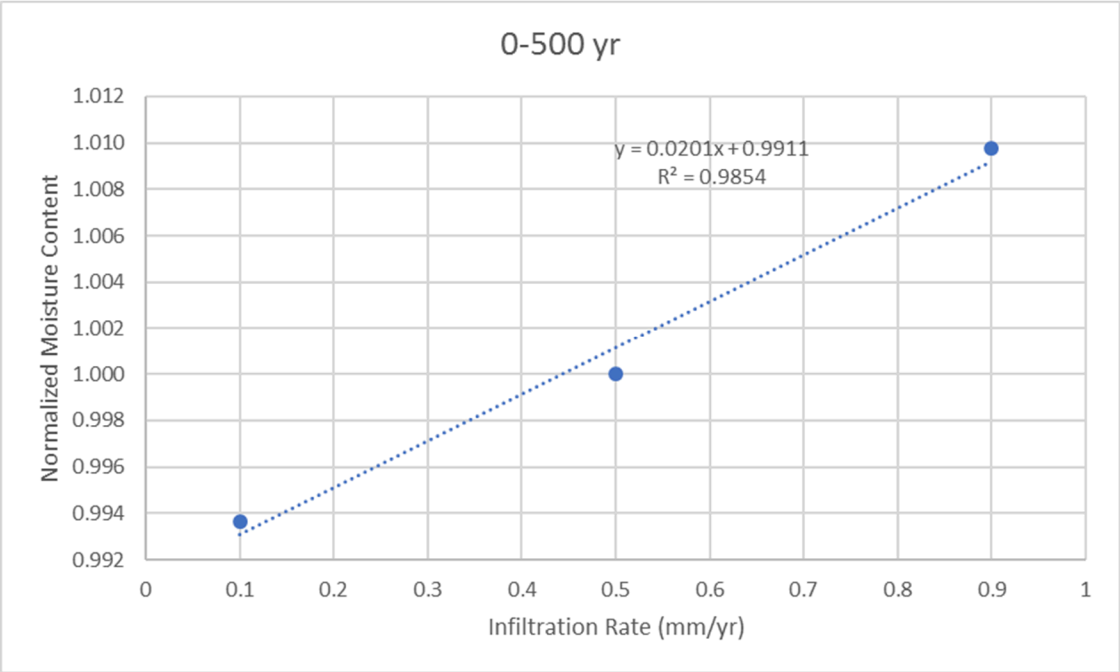


Figure A2-10. Regression Equation for Ratio of Darcy Velocity to the Base Case Darcy Velocity as a Function of Recharge Rate: Degraded Surface Barrier.

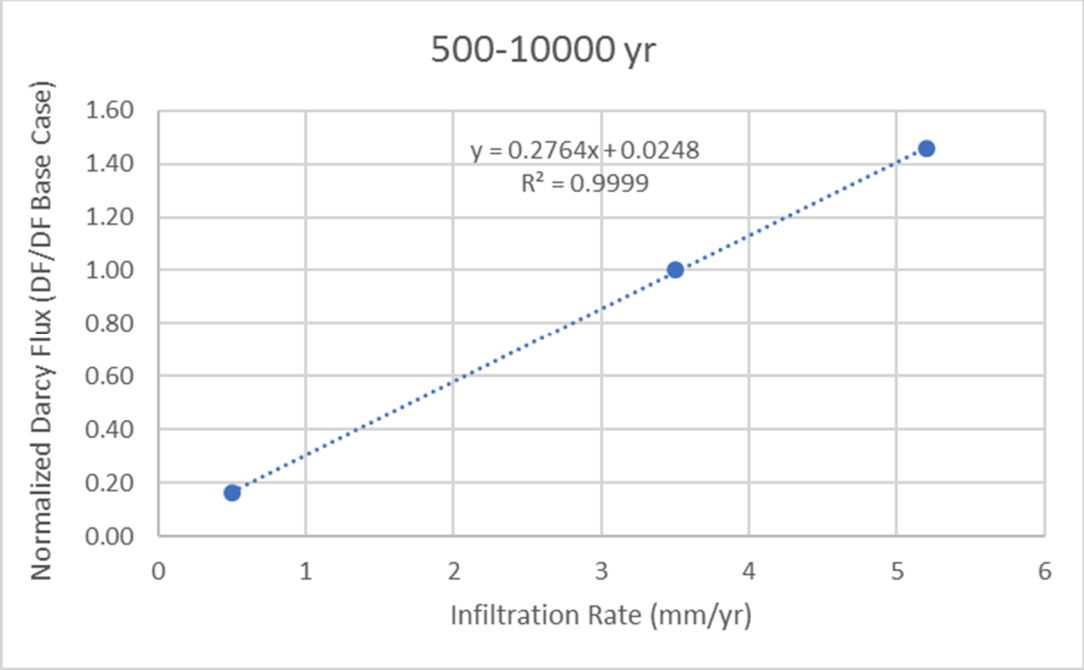
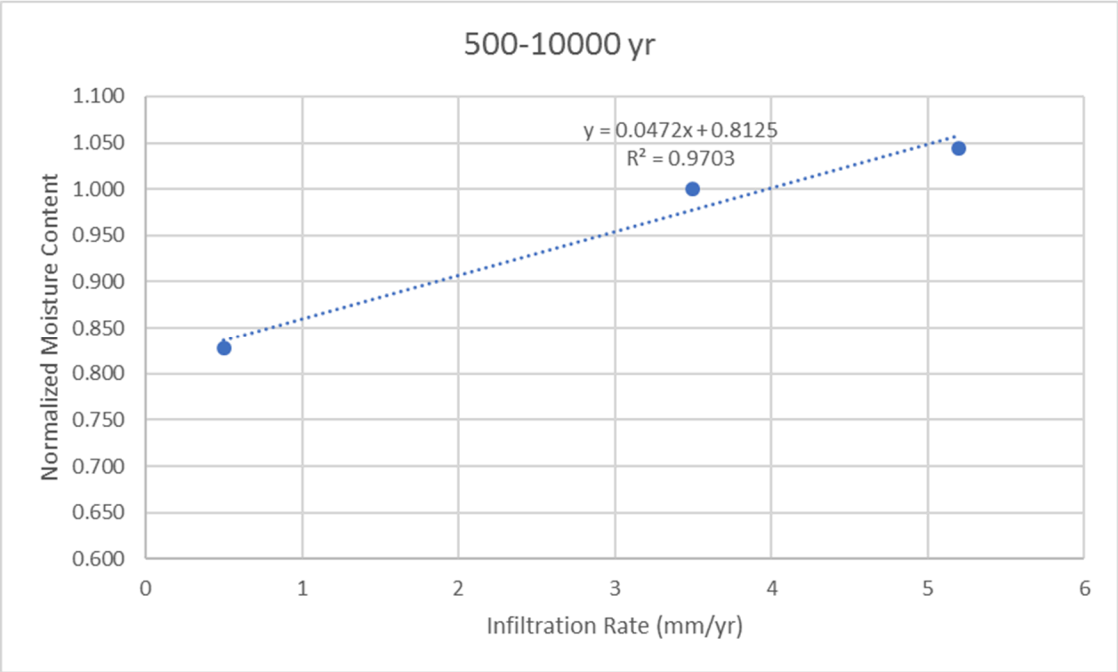


Figure A2-11. Regression Equation for Ratio of Moisture Content to the Base Case Moisture Content as a Function of Recharge Rate: Degraded Surface Barrier.



A2.5 UNCERTAINTY IN SORPTION IN SOILS

The dominant material in the soil column beneath WMA A-AX is sand from the Hanford Formation (referred to as "H2 sand"). Uncertainties in K_d values were developed for H2 sand using a triangular distribution as shown in Table A2-4. The basis for the recommended range for each contaminant is given in the reference provided in the table. The sampled K_d value is then corrected for gravel fraction based on the average gravel content. The same distributions are used for silt sediments of the Cold Creek unit. Distribution coefficients for sand and silt are sampled independently.

Table A2-4. Uncertainty in K_d Values (mL/g) for Sand As a Triangular Distribution. (2 sheets)

Element	Minimum	Most Likely	Maximum	Reference
Ac	100	350	1,500	PNNL-16663
Al	1,500	1,500	1,500	RPP-RPT-46088 (Table 7-10[a])
Am	200	600	2,000	PNNL-17154
B	3	3	3	RPP-RPT-46088 (Table 7-10[a])
C	0	1	100	PNNL-17154
Cd	6.7	6.7	6.7	RPP-RPT-46088 (Table 4-8[b])
Cm	100	350	1,500	PNNL-16663
CN	0	0	0	No relevant information available
Co	0	0	10	PNNL-17154
Cr	0	0	3	PNNL-17154
Cs	10	100	1,000	PNNL-17154
Eu	3	10	100	PNNL-17154
F	0	0	1	PNNL-17154
Fe	25	25	25	RPP-RPT-46088 (Table 7-10[a])
H	0	0	0	PNNL-17154
Hg	52	52	52[c]	RPP-RPT-46088 (Table 7-10[a])
I	0	0.2	2	PNNL-17154
Mn	65	65	65	RPP-RPT-46088 (Table 7-10[a])
Nb	0	0	0.1	PNNL-16663
Ni	1	3	20	PNNL-17154
NO_2	0	0	0.1	PNNL-17154

Table A2-4. Uncertainty in K_d Values (mL/g) for Sand As a Triangular Distribution. (2 sheets)

Element	Minimum	Most Likely	Maximum	Reference
NO_3	0	0	0.1	PNNL-17154
Np	2	10	30	PNNL-17154
Pa	2	10	30	PNNL-17154 (equated to Neptunium)
Pb	3	10	100	PNNL-17154
Pu	200	600	2,000	PNNL-17154
Ra	5	10	20	PNNL-17154
Rn	0	0	0	No relevant information available
Se	0	0.1	3	PNNL-17154
Sm	3	10	100	PNNL-17154 (equated to Lead)
Sn	0	0.5	20	PNNL-17154
Sr	5	10	20	PNNL-17154
Tributyl phosphate	1.89	1.89	1.89	RPP-RPT-46088 (Table 4-8[d])
Tc	0	0	0.1	PNNL-16663
Th	40	300	500	PNNL-16663
U	0.2	0.6	2	RPP-RPT-46088 (Table 4-8)
U_total	0.2	0.8[e]	2	PNNL-17154
Zr	40	300	500	PNNL-16663

References:

PNNL-16663, *Geochemical Processes Data Package for the Vadose Zone in the Single-Shell Tank Waste Management Areas at the Hanford Site*, Table C.5 for chemically-impacted sand sequence.

PNNL-17154, *Geochemical Characterization Data Package for the Vadose Zone in the Single-Shell Tank Waste Management Areas at the Hanford Site*, Table 3.3, for sands with an intermediate-level chemical impact.

RPP-RPT-46088, *Flow and Transport in the Natural System at Waste Management Area C*.

[a] RPP-RPT-46088 obtains distribution coefficient values from The Risk Assessment Information System, Queried 04/17/2019, [RAIS Toxicity Values and Physical Parameters Search, contains chemical and radionuclide toxicity information], https://rais.ornl.gov/cgi-bin/tools/TOX_search.

[b] RPP-RPT-46088 obtains distribution coefficient values from Cleanup Levels and Risk Calculation [CLARC], Queried 04/17/2019, [CLARC Home, contains information to help establish cleanup levels for hazardous waste sites to comply with Model Toxics Control Act cleanup regulation], https://apps.ecology.wa.gov/clarc/CLARCHome.aspx.

[c] The maximum value used in the system model calculations was inadvertently entered as 100 mL/g instead of 52 mL/g. Since Hg is not a dose contributor, the analysis was not re-run with a corrected value for this analysis.

[d] The K_d for tributyl phosphate is used from the cited source without being able to confirm the sources values. Since tributyl phosphate is not a dose contributor, the analysis was not re-run with a verified value for this analysis.

[e] The most likely value used in the system model calculations was inadvertently entered as 0.6 mL/g instead of 0.8 mL/g. Since U was a key contributor to dose, and lower uranium K_d values tend to result in higher doses, the lower value was retained for uncertainty calculations.

A2.6 UNCERTAINTY IN DARCY FLOW IN SATURATED ZONE

As noted in the WMA C performance assessment (RPP-ENV-58782), the flow rate of the unconfined aquifer is a key parameter in the performance assessment. The approach to evaluating uncertainties in the aquifer flow is to define a distribution on the flow rate itself, not on the hydraulic conductivity and aquifer gradient separately. The reason for this is that while the uncertainties in hydraulic conductivity and gradient can be defined, the two are not independent. As a result, it has been found useful to combine the two into a combined uncertainty estimate in Darcy flow rate in the aquifer. This has been implemented as a factor that is multiplied by the base case Darcy flow rate at the upgradient boundary of the WMA A-AX system model.

The foundation for developing the uncertain distribution for Darcy flow rate rests on several observations about the aquifer near WMA A-AX (RPP-RPT-60101).

- Within the resolution of the Central Plateau Groundwater Model, the entire extent of the STOMP© model domain at the water table is represented by Cold Creek groundwater unit (with 18,200 m/d hydraulic conductivity) or by Hanford channel gravel (15,000 m/d hydraulic conductivity). These are effectively the same paleochannel-influenced gravel-dominated hydrostratigraphic unit (HSU). The flow field is generally southeastward with some minor internal variation. For the purposes of the system model, the relevant aquifer unit represented in the model is the Cold Creek unit, with an estimated conductivity of 18,200 m/d.

- At the space scale of the performance assessment, out to the 100-m regulatory boundary, the flow field is essentially uniform, as shown in Figure A2-12. The region of nonuniform flow resulting from the presence of the Ringold A unit (Figure A2-12) are beyond the relevant domain for the performance assessment calculations.

- The uncertainty in the Darcy flux multiplier is dominated by uncertainty in the saturated zone hydraulic conductivity, which varies by more than an order of magnitude. The factor of two uncertainty in hydraulic gradient is comparatively smaller, and was considered to be included within the uncertainty magnitude of Darcy flux.

The basis for the hydraulic conductivity of the unconfined aquifer used in the performance assessment takes account of the accumulated knowledge and experience of many years of study of the aquifer beneath the Central Plateau, undertaken for a variety of purposes by different investigators, using a variety of measurement and modeling approaches. The hydraulic conductivity estimates from various investigations, with focus on the aquifer within the 200 East Area, are presented in Figure A2-13 with the length scale of observation increasing from left to right. The results presented on the left-hand side are from slug tests (small spatial scale measurements), while the pumping test-based measurements are in the middle and the regional scale model-based estimates are on the right-hand side. Where multiple results are provided within a single report that cover slug and pump test data, the range of hydraulic conductivity is shown with a vertical line (Figure A2-13). For the gravel-dominated HSU of interest in the

vicinity of the WMA A-AX, the measured hydraulic conductivity estimates range as high as 51,500 m/day.

The hydraulic conductivity estimates on the left side of Figure A2-13 represent estimates from small-scale tests. The point estimates appear to cluster around 1,000 m/d, and this value is a reasonable representation of the mean values of the vertical lines in the figure as well. As a result, in establishing the uncertain range for the hydraulic conductivity appropriate at the scale of the system model domain, a value of 1,000 m/d has been set as the lower bound. It is noted that this is likely to be an unreasonably low bound for an effective value at this scale. If a substantial region of such low hydraulic conductivity exists beneath WMA A-AX, it would produce observable effects in the hydraulic gradient in the aquifer.

The hydraulic conductivity estimates on the right side of Figure A2-13 are values calibrated from various versions of the Central Plateau Groundwater Model, and are regarded as more reliable estimates for use at the scale of the performance assessment model (see the discussion in RPP-RPT-60101). These estimates allow an upper bound estimate of 21,000 m/d for conductivities in the Hanford formation paleochannel.

To derive the Darcy flow rate multiplier, the saturated hydraulic conductivity range (1,000 to 21,000 m/day) was divided by the best-estimate value (18,200 m/day) and a triangular distribution was chosen with the following parameters:

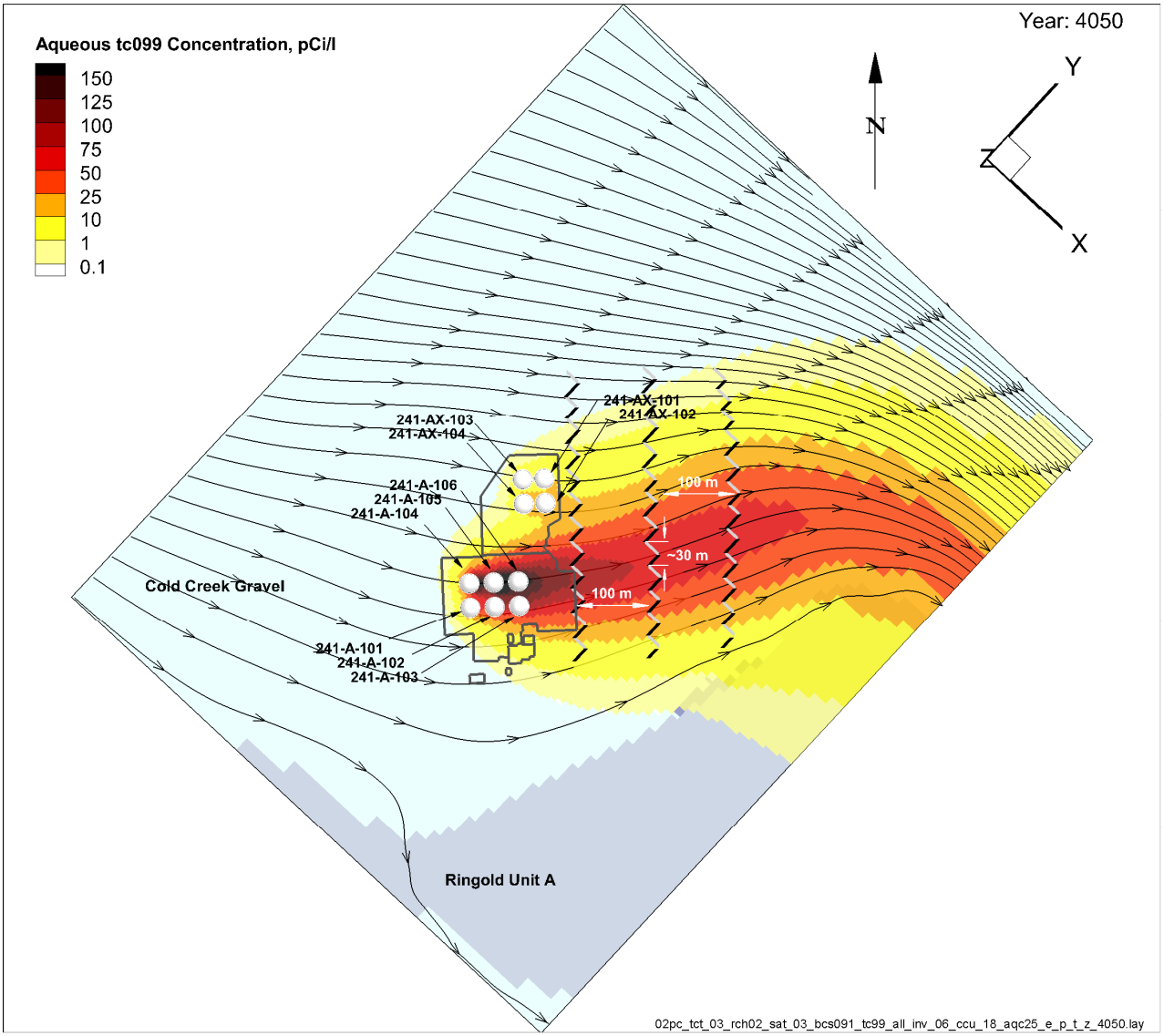
- Minimum = 0.05
- Most Likely = 1
- Maximum = 1.2.

A2.7 UNCERTAINTY IN DISPERSIVITY

A2.7.1 Vadose Zone Dispersivity

In unsaturated media, the longitudinal dispersivity is dependent on soil moisture content (or matric potential) and differs when the primary flow and transport is parallel to the bedding plane versus being primarily perpendicular to the bedding. Multiple lines of evidence were presented in RPP-ENV-58782 Appendix B on the estimation of dispersivity for WMA C. The conclusion was that the best estimate coincided with the lower bound of the range of dispersivity. This means that the base case represents a lower (conservative) bound for this parameter. As a result, this parameter has been fixed at its base case value of 25 cm for the current uncertainty analysis, and it not assigned a parameter distribution.

Figure A2-12. Waste Management Area A-AX Process Model Analysis of Technetium-99 Concentration in Groundwater from All Sources at the Approximate Time the Maximum Concentration Occurs.

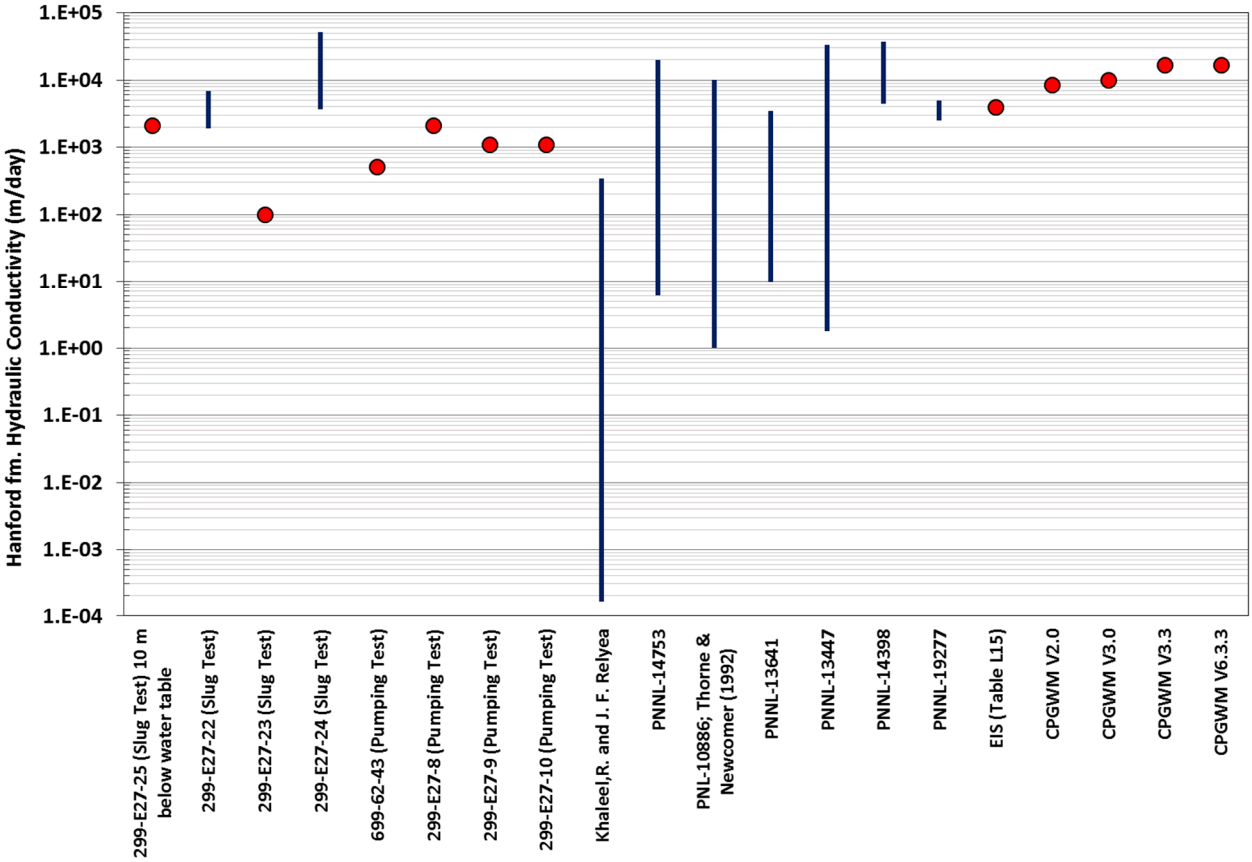


Reference: RPP-CALC-63164, *WMA A-AX Performance Assessment Contaminant Fate and Transport Process Model to Evaluate Impacts to Groundwater*.

A2.7.2 Saturated Zone Dispersivity

The dispersivity parameter in the one-dimensional GoldSim© model represents the longitudinal dispersivity. Given the rapid flow rates and short transport pathway in the saturated zone, results are anticipated to be insensitive to this parameter. As a result, this parameter has been fixed at its base case value of 10.5 m for the current uncertainty analysis, and it not assigned a parameter distribution.

Figure A2-13. Hanford Formation Saturated Hydraulic Conductivity Estimates Based on Slug Tests, Pump Tests, and Model Calibration.



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APPENDIX B

SCRIPT FOR RANDOM FOREST ANALYSIS IN R

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B1.0 INTRODUCTION

The Random Forest analysis discussed in Section 7.6.2.2 was performed using the script documented in this Appendix.

Random Forest Script

```
setwd("U:/A_AX/uncert")
#library(time)
library(randomForest)
indata=read.table(file="MAX_DOSE_300_REL_10000YR.txt",header=TRUE)
nvarx = 128
x=indata[,2:nvarx]
y=indata[,1]
#old <- getTime()
ilv.rf=randomForest(x,y,importance=TRUE,ntree=1000)
#timeElapsed( old, new = getTime() )
#timeChar( time = getTime() )
#timeReport(old)
write.table(importance(ilv.rf),file="iyearx rf relinf.txt",quote=FALSE)
partialPlot(ilv.rf,indata,Darcy_Flux_Mult_SZ)
#
```

ATTACHMENT 1

INSTALLATION and CHECKOUT FORM

CHPRC SOFTWARE INSTALLATION AND CHECKOUT FORM

Software Owner Instructions:

Complete Fields 1-13, then run test cases in Field 14. Compare test case results listed in Field 15 to corresponding Test Report outputs. If results are the same, sign and date Field 19. If not, resolve differences and repeat above steps.

Software Subject Matter Expert Instructions:

Assign test personnel. Approve the installation of the code by signing and dating Field 21, then maintain form as part of the software support documentation.

GENERAL INFORMATION:

1. Software Name: GoldSim Pro Software Version No.: 12.0

EXECUTABLE INFORMATION:

2. Executable Name (include path):

[redacted]\GoldSim.exe

3. Executable Size (bytes): 2,836 KB

COMPILATION INFORMATION:

4. Hardware System (i.e., property number or ID):

Compiled by vendor

5. Operating System (include version number):

Windows (compiled by vendor)

INSTALLATION AND CHECKOUT INFORMATION:

6. Hardware System (i.e., property number or ID):

WF40244

7. Operating System (include version number):

Windows 10 Enterprise version 1709 build 16299.1029

8. Open Problem Report? ◉ No ○ Yes PR/CR No.

TEST CASE INFORMATION:

9. Directory/Path:

[redacted]General Examples

10. Procedure(s):

per CHPRC-00224 Rev 1, GoldSim Pro Software Test Plan

11. Libraries:

N/A

12. Input Files:

FirstModel.gsm

13. Output Files:

FirstModel.gsm

14. Test Cases:

GS-ITC-1

15. Test Case Results:

Match expected results as presented in CHPRC-00224, GoldSim Pro Software Test Plan

16. Test Performed By: Kearn Patrick Lee

17. Test Results: ◉ Satisfactory, Accepted for Use ○ Unsatisfactory

18. Disposition (include HISI update):

None.

CHPRC SOFTWARE INSTALLATION AND CHECKOUT FORM (continued)

1. Software Name: GoldSim Pro Software Version No.: 12.0

Prepared By:

19.	WILLIAM NICHOLS (Affiliate) Digitally signed by WILLIAM NICHOLS (Affiliate) Date: 2019.03.21 06:43:16 -07'00'	WE Nichols	
	Software Owner (Signature)	Print	Date

20. Test Personnel:

	Kearn Patrick Lee	3/18/19
Sign	Print	Date
Sign	Print	Date
Sign	Print	Date

Approved By:

21.		N/R per SMP	
	Software SME (Signature)	Print	Date

ATTACHMENT 2

SYSTEM MODEL CHECKING LOG

CHECKER LOG FOR SYSTEM MODELS

Project and Environmental Model Calculation Specific Information:

Project: T2C25, WMA A-AX Performance Assessment

Responsible Manager or Designee, and Position: Bob Hiergesell, Technical Lead

Originating Group or Department: Closure and Interim Measures | Date: 5/30/2019

Environmental Model Calculation File Report and Revision No.: RPP-CALC-62541 Rev. 0

Environmental Model Calculation File Title: WMA A-AX Performance Assessment Uncertainty Calculation

Check: Environmental Model Calculation File Document Elements

	List where Information is Described *(EMCF Section Number)*	Is the Description Correct and Sufficient?			Checker Signature
		Yes	No	If No, describe deficiency:	
Purpose	1.0	◉	○		
Calculation Approach	3.4	◉	○		
Assumptions	4.1	◉	○		
Inputs *(reference detailed checklist below as well)*	4.2	◉	○		
Equations used	7.1	◉	○		
Conclusions	7.7	◉	○		
References	8.0	◉	○		

Check: Controlled Software Use

	List where Information is Described *(EMCF Section Number)*	Is the Criteria Met?			Checker Signature
		Yes	No	If No, describe deficiency:	
Software used in the calculation is appropriate for application	5.1	◉	○		
Software use is approved and properly validated in accordance with approved software management plan	5.4	◉	○		
Software use is properly documented	5.2	◉	○		
Verify data was input correctly to approved software or spreadsheets	Appendix A	◉	○		
If a spreadsheet is used, verify inputs/outputs of calculation(s) to ensure accuracy	Spreadsheets were used in output and checked.	◉	○		

Check: Perform Calculation to Verify Free of Errors

	Describe how calculation was performed	List any discrepancies encountered *(If none, enter "None")*	Checker Signature
Perform the environmental model calculation as described to verify it is free of errors	100-realization was performed	None	

CHECKER LOG FOR SYSTEM MODELS (Continued)

Check: Process Model Parameterization *(Specify Values and Units in Each Column)*

Model Parameter Type	(1) Input Documented in EMCF?	(2) Values checked against parameter source?	(3) Input in EMCF matches model input file(s)?
Simulation duration	Yes	Yes	Yes
Simulation time step control	Yes	Not applicable	Not applicable
Simulated chemical list	Referenced System Model MPR	Not applicable	Not applicable
Simulated radionuclides list	Yes	Yes	Yes
External model components identified and documented or referenced	No	Not applicable	Not applicable
External model linkages *(dynamic link libraries, etc.)* checked	No	Not applicable	Not applicable
If model is probabilistic, stochastic distributions are defined and consistent	Yes	Yes	Yes
Input units are declared and of correct dimensionality	Yes	Yes	Yes
Equations used in the model file are presented in EMCF and consistent	Yes	Yes	Yes

Check: Further Checks *(Record additional checks performed and results)*

Model Parameter Type	(1) Input Documented in EMCF?	(2) Values checked against parameter source?	(3) Input in EMCF matches model input file(s)?
Inventory: Radiological Decay Correction. Does the inventory *(source term)* include radionuclides, and if so, is it decay-corrected to the appropriate date for inclusion as a source?	It is decay-corrected. Not documented but referenced the system model MPR.	Inventory data used in results presentation (fractional cumulative release)match the source	Not applicable.
Inventory: Mass Balance. Is mass balance of inventory maintained in system model calculation(s)?	Not applicable	Not applicable	Not applicable