EXECUTIVE SUMMARY

Under the direction of the U.S. Department of Energy (DOE), Hanford Site contractors are engaged in the world's largest environmental cleanup project. CH2M HILL Hanford Group, Inc. (CH2M HILL) is the closure contractor for the DOE Office of River Protection, providing planning, project delivery, and nuclear safety expertise to accelerate clean up and closure of the Hanford Site's 177 underground waste tanks. The tasks performed in this effort provide a technical basis for remediation and site closure decisions.

The Remediation and Closure Science (RCS) Project at the Pacific Northwest Laboratory is funded through DOE Richland Operations. The RCS Project develops data, methods, and tools to determine contaminant inventory; contaminant transport in the vadose zone, groundwater, and river; and to predict ecological impacts. These data and knowledge are required to make decisions regarding remediation and closure of waste sites and to develop final remedies for groundwater contamination. Among the various tasks in this project is one to develop a Soil Inventory Model (SIM), which is a probabilistic approach to estimate the inventory of contaminants that were released to the soil during the Hanford Site production mission. This document provides the latest description of SIM, Rev. 1, published in collaboration with CH2M HILL.

SIM is an extension and enhancement of previous efforts to quantify contaminant inventories in the Hanford Site waste storage tanks. In the 1990s, the Hanford Defined Waste (HDW) Model was used to predict what was in the single- and double-shell tanks at the Hanford Site. The data gathered as part of that modeling effort included fuel processed, chemical process knowledge, and waste transfer information. The HDW Model also made an initial attempt to define what was disposed to the ground. The SIM Rev. 1 effort provides more details of what went into specific waste sites other than the tanks and provides a more complete picture of these discharges. Like the HDW Model, much of SIM is based on historical records and data from the Hanford Site’s various process facilities that extracted plutonium and uranium from spent nuclear fuel. Data from samples collected from selected high-level waste tanks and from process control data contained in historical waste management documents were used to update the HDW Model composition estimates used in SIM Rev. 1.

SIM Rev. 1 can be used to provide insight into contaminated soil inventories associated with the liquid waste disposal sites, unplanned releases, and tank leaks at the Hanford Site and their associated uncertainty. This information leads to more effective use and application of remediation resources by allowing risk-based priorities to be established.

SIM generates inventory and uncertainty estimates for 46 radionuclides and 29 chemicals using 196 waste streams applied to 377 liquid-waste disposal sites, unplanned releases, and tank leaks over their operating lifetimes in intervals of one year, from 1944 to 2001. The operating times for these sites varied from several weeks to decades in length and could consist of multiple waste streams. These calculated estimates provide uncertainty bounds around the mean inventories as part of a Monte Carlo calculation using uncertainties defined in the input data.

This is the first time formal, comprehensive estimates of uncertainty have been generated for the inventory from liquid waste disposal sites, unplanned releases, and tank leaks. The total predicted mean volume for the selected liquid waste disposal sites is ~1,023,000 megaliters (ML). The overall mean volume for the tank leaks is estimated at 2.18 ML, and for the various unplanned release sites, the mean loss volume is estimated to be 3,419 ML. For comparison, the underground storage tanks at the Hanford Site contain approximately 200 ML of waste.

Although approximately 70% of the selected analyte results are within the SIM predicted 0.5 to 99.5 percentile range, this metric may be considered too broad to be considered agreement between SIM and the reference data. Further evaluations using narrower criteria may be justified to better describe model performance. Currently, the methods and assumptions used to represent the mean values and evaluate uncertainties in this revision of the model are considered coarse but realistic. In evaluating the data, the size of the uncertainties associated with these estimates are significant, spanning in some cases an order of magnitude or more. This condition does not necessarily represent a deficiency in the data; all that can be inferred is that the system has a substantial amount of intrinsic uncertainty and that any decisions made must take this feature into account.

The principal factor influencing the model output is the degree to which reliable quantitative descriptions could be provided for the inputs. To further reduce the estimated uncertainty using SIM, additional information regarding the input distributions is needed. Model assumptions and constraints associated with computer software coding and the number of trials performed in the analysis removed many of the irregularities associated with the individual process batches and smoothed the variation observed in source documentation for the waste sites. The largest contributors to uncertainty in the estimated inventories were sparse data with broad uncertainties used to quantify analyte behavior or where simple distributional assumptions were used generally, at relatively fine levels of resolution, to quantify analyte behavior. This condition is especially true for individual realizations (e.g., annual results) for several radionuclides reported in SIM because of large production uncertainties derived from ORIGEN2 output. However, the uncertainties at more summary levels of evaluation (e.g., total inventory over the operating history) were more constrained and did not span as wide a range (in a relative sense) as was observed at the level for an individual year.

Limited data are available to estimate waste site inventories for many waste sites. Consequently, waste sites with no basis for waste composition often used data that had been applied to nearby sites. These waste sites operated in a similar time frame and are expected to have the same composition, because waste management practices at the Hanford Site often segregated waste in predictable ways, and wastes were often specific to a particular time and production plant. This feature sometimes resulted in a small number of sites containing the majority of a number of analytes of interest. In SIM Rev. 1, the top ten sites by inventory for a particular analyte account for between 39% and 100% of the total mass/activity for that analyte.

The number of sites and greater time-scale resolution in SIM Rev. 1 is larger than that predicted with the previous version of SIM (88 sites evaluated using 16 waste streams over an assumed one-year period for a waste site). SIM was revised and refined to correct several assumptions

regarding waste stream solubility and composition as well as the default assumption for uncertainty used in the proof-of-principle evaluation. These changes improved the overall technical basis of the estimates, and this report supersedes the data and report presented in the first SIM effort.

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LIST OF TERMS

Abbreviations and Acronyms

CB	Crystal Ball®
cCDI	compare Cumulative Decayed Inventory
CDI	Cumulative Database Inventory
CH2M HILL	CH2M HILL Hanford Group, Inc.
DOE	U.S. Department of Energy
ETF	Effluent Treatment Facility
HDW	Hanford Defined Waste
ITS	in-tank solidification
LHS	Latin Hypercube Sample
Misc	miscellaneous
N/A	not applicable
NRDWL-BC	Non-radioactive Dangerous Waste Landfill—BC cribs
OCB	Open Crystal Ball®
PFP	Plutonium Finishing Plant
PUREX	Plutonium-Uranium Extraction (Facility)
QA	Quality Assurance
RCS	Remediation and Closure Science
REDOX	Reduction-Oxidation (Facility)
RG	Rubber Glove Line (Process)
RPD	relative percent difference
RSD	relative standard deviation
SAC	System Assessment Capability
SIM	Soil Inventory Model
SMM	Supernatant Mixing Model
StdDev	Standard Deviation
Sup Vol	supernatant volume
TBP	tributyl phosphate
UNH	uranyl nitrate hexhydrate
UPR	unplanned release
WIDS	Waste Information Data System
WM	Waste Management
WSWB	Waste Stream Workbook
WTP	Waste Treatment and Immobilization Plant

Units

Ci	Curies
ft	feet
g	grams
g/kg	grams per kilogram
g/mL	grams per milliliter
gal	gallons
hr	hour
kCi	kiloCuries
kg	kilograms
kgal	kilogallons
L	liters
m	meters
MB	megabytes
ML	megaliters
mL	milliliters
pCi	picocuries
μCi/g	microcuries per gram
μg/g	micrograms per gram

LIST OF WASTE TYPE TERMS

This section lists the waste type definitions used from Revision 5.0 of the HDW Model (Higley et al. 2004).

BISMUTH PHOSPHATE PROCESS WASTE TYPES (1944-1956)

Waste Type	Definition
MW1	$BiPO_4$ Metal Waste (1944-1949)
MW2	$BiPO_4$ Metal Waste (1950-1956)
1C1	$BiPO_4$ First cycle decontamination waste and coating waste (1944-1949)
1C2	$BiPO_4$ First cycle decontamination waste and coating waste (1950-1956)
2C1	$BiPO_4$ Second cycle decontamination waste (1944-1949)
2C2	$BiPO_4$ Second cycle decontamination waste (1950-1956) and low activity cell 5-6 drainage waste (June 1951-1956)
224-1	Lanthanum fluoride process 224 Building waste (1944-1949)
224-2	Lanthanum fluoride process 224 Building waste (1950-1956)

URANIUM RECOVERY AND SCAVENGING WASTE TYPES (1952-1958)

TBP	Tributyl phosphate process waste (1952-1958), same as UR
PFeCN1	Ferrocyanide sludge from TBP in-plant scavenged supernatant and co-disposed TBP sludge (1954-1955)
PFeCN2	Ferrocyanide sludge from TBP in-plant scavenged supernatant and co-disposed TBP sludge (1955-1958)
TFeCN	Ferrocyanide sludge from supernatant scavenging in 244-CR Vault (1955-1958). These supernatants consisted of TBP supernatant and the commingled supernatants from other wastes stored in the same tanks
1CFeCN	Ferrocyanide sludge from in-plant scavenging of T-Plant 1C waste (without coating waste). Transferred to TY-Farm (1955-1956)

REDUCTION AND OXIDATION (REDOX) PROCESS WASTE TYPES (1952-1966)

R1	REDOX high-level waste (1952-1958)
R2	REDOX high-level waste (1959-1966)
CWR1	REDOX cladding waste, aluminum clad fuel (1952-1960)
CWR2	REDOX cladding waste, aluminum clad fuel (1961-1966)

PLUTONIUM-URANIUM EXTRACTION (PUREX) PROCESS WASTE TYPES (1956-1990)

P1	PUREX high-level waste (1956-1962)
P2	PUREX high-level waste (1963-1967)
P2'	PUREX acid waste to B-Plant (1964-1972)
P3AZ1	PUREX high-level waste to AZ-101 (1983-March 13, 1986)
P3AZ2	PUREX high-level waste to AZ-102 (March 13, 1986 to 1990)

CWP1	PUREX cladding waste, aluminum clad fuel (1956-1960)
CWP2	PUREX cladding waste, aluminum clad fuel (1961-1972)
CWZr1	PUREX (and REDOX) zirconium cladding waste, (1968-1972)
CWZr2	PUREX zirconium cladding waste (1983-1989)
OWW1	PUREX organic wash waste and non-boiling waste (1956-1962)
OWW2	PUREX organic wash waste and non-boiling waste (1963-1967)
OWW3	PUREX organic wash waste (1968-1972)
PL1	PUREX non-boiling waste (1968-1972)
PL2	PUREX organic wash waste and non-boiling waste (1983-1988)
TH1	Thoria process wastes (1966)
TH2	Thoria process wastes (1970)
PASF	PUREX Ammonia Scrubber Feed

CESIUM AND STRONTIUM RECOVERY WASTE TYPES (1961-1985)

HS	Hot Semiworks strontium purification waste (1961-1968)
AR	Water washed PUREX sludge entrained in decants of recovered sludge or the water washes of this sludge and the solids remaining after acidification (1967-1976)
B	B-Plant high-activity waste – Rare earth (RE) fission products, recovered current acid waste (CAW), solvent wash waste, and any solution containing high activity (including cask station receipts, cell drainage containing product spills) (1967-1972)
BL	B-Plant low-activity waste – 1AW solvent extraction waste stream (includes complexants added for solvent extraction), the 1CP/organic wash waste during PAS processing, and insoluble solids remaining after treatment of solids centrifuged from CAW feed (i.e., acid leached and water washed PUREX high-level waste [HLW] sludge). Cell drainage and Waste Encapsulation Storage Facility (WESF) transfers with low radionuclide content (1967-1976)
SRR	High-activity waste from B-Plant processing of PUREX acidified sludge (PAS), solids centrifuged from AR vault feed, strontium purification wastes after solvent extraction (SX), RE or ion exchange (IX) rework, and other solutions containing activity (including cask station receipts, cell drainage containing product spills, WESF returns unsuitable for rework and crude RE disposal). (1969-1985)
CSR	Supernatants from which the cesium has been removed by ion-exchange. 241-C-801 cask station (1962-1967). B-Plant Waste Fractionization (1967-1976).

OTHER PROCESS FACILITY WASTES

Z	Plutonium Finishing Plant waste (1974-1988)
DW	Decontamination wastes, primarily from T Plant operations (1967-1976)
N	N Reactor decontamination waste (1976-1990)

MISCELLANEOUS WASTES

CEM	Portland cement added to tank 241-BY-105
DE	Diatomaceous earth added to six tanks (241-BX-102, 241-SX-113, 241-TX-116, 241-TX-117, 241-TY-106, and 241-U-104)
NIT	Partial neutralization feed for evaporator campaigns (1977-1981)

SALTCAKES AND SALT SLURRIES

BT-SltCk	Saltcake from 242-B Evaporator operation (1951-1953) and the 242-T Evaporator operation (1951-1955). Formerly BSltCk and T1SltCk.
BYSltCk	Saltcake from in-tank solidification (ITS) in BY-Farm (1965-1974)
RSltCk	Saltcake from self-concentration in S- and SX-Farms (1952-1966)
T2SltCk	Saltcake from the last 242-T Evaporator campaign (1965-1976)
A1SltCk	Saltcake from the first 242-A Evaporator campaign using 241-A-102 feed tank (1977-1980)
A2SltCk	Saltcake form the second 242-Evaporator campaign using 241-AW-102 feed tank (1981-1988)
S1SltCk	Saltcake from the first 242-S Evaporator campaign using 241-S-102 feed tank (1973-1976)
S2SltCk	Saltcake from the second 242-S Evaporator campaign using 241-SY-102 feed tank (1977-1980)

1.0 INTRODUCTION

The Hanford Soil Inventory Task is part of the U. S. Department of Energy's (DOE's) Remediation and Closure Science (RCS) Project underway at Pacific Northwest National Laboratory. Staff involved in this task are developing and applying a mass balanced method to estimate the inventory of contaminants, together with their associated uncertainties, disposed to soil waste sites. Development of this method resulted in the Soil Inventory Model (SIM) and its associated output presented in this document.

The Soil Inventory Task builds on existing information to develop models, such as SIM, capable of estimating the overall Hanford Site inventory with uncertainties. The System Assessment Capability (SAC) (Bryce et al. 2002) and other Hanford Site projects use the results of these models in their waste management, risk assessment, and remediation efforts. This report describes the project requirements, computing architecture, and features; input data sources/modeling assumptions; calculation method, output description and organization; and results, analysis, and conclusions. The information in this report is of a technical nature and is intended to provide a scientific discussion of the SIM Rev. 1 model.

1.1 OBJECTIVE OF THE REMEDIATION AND CLOSURE SCIENCE (RCS) PROJECT

The objective of the RCS Project is to provide new knowledge, data, tools, and the understanding needed to make sound remediation decisions. The RCS Project is focused on resolving key technical issues that help inform and influence remediation decisions and decisions that impact the closure of the Hanford Site, in partnership with SAC, the Groundwater Remediation and Soil Waste Site Projects at Fluor Hanford, Inc. and the Tank Farm Vadose Zone Project at CH2M HILL Hanford Group, Inc. (CH2M HILL).

1.2 OBJECTIVES OF THE SOIL INVENTORY TASK

The objective of the Soil Inventory Task is to develop a probabilistic approach to estimate mass balanced-based (i.e., holistic) inventories for the Hanford Site post-closure setting. This approach is needed to support SAC and has also been useful to other Hanford Site remediation projects.

The effort with regard to the vadose zone is focused on extending the Hanford Defined Waste (HDW) Model (Agnew et al. 1997a; Higley et al. 2004) and other process knowledge to quantify inventories and uncertainties of liquid waste disposal sites; unplanned releases and tank leaks that directly received process waste in the 200 Areas of the Hanford Site; and a select number of sites in the 300 Area. The result of this effort was SIM. Waste streams from the chemical separations conducted in the canyon buildings were discharged purposefully and directly to a variety of waste sites such as ditches, ponds, chemical sewers, and cribs. In addition, as a result of past waste management practices, waste from the high-level waste tanks was disposed to the

ground through specific retention cribs and trenches. Other waste sites were the result of inadvertent discharges either from unplanned releases (e.g., overfilling tanks, piping breaches, other miscellaneous infrastructure failures) or from tank farm leaks.

1.3 SCOPE

The scope of activities for fiscal year (FY) 2005 was to provide comprehensive chemical and radionuclide inventories and uncertainties for a variety of liquid waste disposal sites, unplanned releases, and tank leaks as a function of time using SIM, Rev. 1. These estimates present a statistical description of the inventories for these sites and, thus, consist of a mean, median, standard deviation about the mean, and several percentiles for each analyte for each year of operation. Additionally, waste site analyte disposal concentrations and volumes as a function of time are provided. These waste sites have been grouped geographically and/or by facility use into 20 Operable Units/Closure Zones for purposes of analysis and evaluation at more general levels of resolution. Appendix A describes the membership of the various operable units/closure zones evaluated.

There are several substantial differences between SIM Rev. 0 and SIM Rev. 1. Because SIM Rev. 0 was a proof-of-principle effort (Simpson et al. 2001), the model was modest in scope and relatively straightforward. The initial SIM used a combination of HDW Model Rev. 4 (Agnew et al. 1997a) and historical data regarding analytes, waste streams, and significantly simplified assumptions. Only 16 waste streams were used to describe the waste stream inputs to the disposal sites. The uncertainty distributions selected to represent the waste stream conditions were highly constrained (normal, lognormal, or triangular), often based on limited data, and not unusually large in magnitude.

These numerous simplifying assumptions were used in SIM Rev. 0 to calculate inventory and uncertainty. For example, placeholder values used to estimate the unmeasured radionuclide uncertainties were used until a defensible technical rationale for deriving those uncertainties was developed. Compared to Rev. 1, these placeholder values substantially underestimated the uncertainty associated with these analytes. Furthermore, the site disposal volumes were often simplified (reduced in the number of contributing waste streams, especially with regards to quantifying tank farm leak events) and consolidated as a function of time. The total inventories for a site were represented using a one-year operating history as a simplifying approximation. The 88 sites were modeled as separate groups according to their definition (disposal site, unplanned release, or tank leak) to ease comparisons during data analysis. The data output for the modeled sites was also relatively modest (approximately 60 MB), with all site results able to fit on one worksheet.

SIM Rev. 1 is a significantly larger and more ambitious model than SIM Rev. 0. The inventory estimates for 377 waste sites for 75 analytes are provided stochastically over the operating life of the waste site. These site inventories are reported as a function of time for each analyte in one-year increments. Because of the increase in size, model run times became much longer, requiring several days of computing time. To address this challenge, a method for distributed computing and calculation was developed. In addition, some substitutions and additions were made about the sites and chemicals modeled and reported: silver replaced chemical strontium

and tributyl phosphate (TBP) replaced dibutyl phosphate (DBP), and carbon tetrachloride and ferrocyanide were added to the list of analytes. Certain tank farm leaks and unplanned releases were removed because insufficient data were available to support inventory estimates. Additionally, substantial revisions to the HDW Model were made (Higley et al. 2004), including decay of all radionuclides to January 1, 2001, resulting in much different waste descriptions. Finally, a new, consistent uncertainty definition method was developed and applied to the various radionuclides quantified by SIM.

All of the sites, regardless of category, were modeled together in SIM Rev. 1, with results organized by operable unit. Internal checking routines, comparisons to reference values, comprehensive data analysis, and model performance metrics at various levels of resolution were included in this version. Thus, the data output for a single model run was much larger than the previous version (approximately 650 MB), requiring multiple worksheets for reporting. Additional model runs for software quality assurance (QA) and model convergence requirements also adds substantially to the amount of data associated with the final results.

Because of the large quantity of data generated (and the corresponding amount of paper necessary to print it—several thousand pages), the inventory estimates and the supporting appendices are presented in electronic attachments to this report. The output results will also be placed into an electronic database (such as the tank characterization database) for retrieval and configuration control.

2.0 REQUIREMENTS

A computer model capable of calculating inventories and uncertainties as a function of time was specified to address the needs of the RCS Project. The ability to use familiar, commercially available software on a high-performance personal computer for data input, modeling, and analysis rather than custom software on a workstation or mainframe computer for modeling was desired. A description of the general method, hardware, software, and QA specifications is provided in this section. Additional discussion of project requirements and more comprehensive QA data analysis is provided in Appendix B.

2.1 METHOD SELECTION

As previously noted, the objective of this task is to provide an approach to estimate mass balanced inventories with uncertainties for the Hanford Site post-closure setting. Because of this requirement, researchers selected a stochastic simulation (a Monte Carlo-type calculation) to provide estimates of inventory and uncertainty. Stochastic simulation was chosen because the modeling parameters for this calculation did not have satisfactory closed-form definitions to approach the problem from a purely mathematical standpoint; the available waste stream/site data were not sufficiently comprehensive to apply regression analysis; and the desire for a comprehensive description of uncertainty eliminated sensitivity analysis as potential methods.

Stochastic simulation is a broadly accepted modeling technique that meets the requirements of the task. Furthermore, there are substantial resources available to its application in practice; therefore, this method was used in developing SIM. In this approach, several options were considered for model development and the Open Crystal Ball®[1] (OCB) statistical package (Decisioneering 2002) was selected. It provided an appropriate development platform for construction of SIM.

2.2 SOFTWARE

The software required to execute the model includes an operating system with .NET® (dot NET) capability, such as Windows®[2] XP, the developed interface application software, Microsoft®[3] Excel, and the OCB statistical package (Decisioneering 2002). The .NET® provided the environment for OCB and the interface application to work with the Excel input workbook. The same Excel workbook that is the location of the input data was also used in reporting a summary of the final results. SIM also generates a series of workbooks reporting the comprehensive results for each site in each identified operable unit.

[1] Open Crystal Ball® is a registered trademark of Decisioneering, Inc., Denver, Colorado.
[2] Windows® is a registered trademark of Microsoft Corporation, Redmond, Washington.
[3] Microsoft® is a registered trademark of Microsoft Corporation, Redmond, Washington.

2.3 HARDWARE

Operation of SIM is limited by the amount of available random access memory (RAM) provided in the computer. However, because Windows® XP constrains the RAM memory use to 1.3 Gigabytes (GB), more RAM above this limit does not enhance performance. Because run-time performance is a major constraint for models of this type, several design approaches were examined to optimize the speed of the simulation with regard to the available computing resources. A distributed computing feature was developed; thus, several computers with at least a 2.0 GHz processor and 2 GB of RAM are recommended to run SIM and complete the simulations with a reasonable run-time (unless exploratory analyses are being performed that do not require converged model results).

2.4 QUALITY ASSURANCE

A standard practice for developing models of this type includes a QA element to establish that the technical rigor used in modeling was sufficient in addressing the demands of the task. This QA element (commonly known as verification and validation) generally has two purposes:

1. The first purpose is to determine the software and model suitability for the intended task (e.g., is the model describing the problem properly and is the software performing the desired mathematical operations correctly?).
2. The second purpose is to establish that the results produced by the software and model are consistent and repeatable within an acceptable tolerance and agree with observation. An additional element in this case is to demonstrate that the Latin hypercube modeling parameters selected for the Monte Carlo analysis do not impart a bias or otherwise adversely affect the outcome of the model.

Verification and validation testing, convergence testing, and bin size evaluation have all been performed. The results from this QA and verification/validation testing effort can be found in Appendix B. A brief description of the results of the QA testing is contained in the following sections.

2.4.1 Software Validation and Verification

Open Crystal Ball® for .NET (OCB.Net) was used to generate the randomized values within the limits of a defined distribution for an input assumption and to calculate the results of the model. Validation and verification of the OCB software was performed to ensure that the distributions were computed properly and those calculations were being performed correctly. Test files using example distributions with known results were used to examine the software algorithms. The results from these test files have confirmed that the dynamic linked library for OCB used in SIM provides statistically indistinguishable values (to within approximately 0.3% difference) to S-PLUS®[4] with test files using example distributions similar to those used in this model. Results from this dynamic linked library have also been compared to the released version of OCB, which

[4] S-PLUS® is a registered trademark of Insightful Corporation, Seattle, Washington.

is used as an add-on to the Excel application. Because of these verification and validation testing results, the values produced with this version of OCB.Net are considered reliable.

2.4.2 Monte Carlo Convergence Test Results

In order to determine if the SIM results are consistent and repeatable, convergence testing was performed on a series of models run using varying numbers of trials. Because the power of a Monte Carlo model increases as a function of the square root of the number of trials, models were run at 1,000, 2,500, 5,000, 10,000, and 25,000 trials and the outputs evaluated. Using empirical results from a test file designed to represent the most extreme combinations of distributions available in SIM, the number of trials to be used in an evaluation was determined to be approximately 25,000, and the model must be run under Latin hypercube sampling to be satisfactorily converged.

The convergence criterion for SIM was set at this threshold: no more than 5% of the individual analyte results could have deviations greater than 5%, using a maximum trial-to-trial variation on the mean, median, standard deviation, the fifth percentile and the ninety-fifth percentile. Certain allowances were made for biases resulting from evaluating very small numbers (in this case, values less than 1E-12). This criterion established a ninetieth percentile range that was used as a standard metric for convergence evaluation. The results from these trials demonstrate that the model as defined provides reproducible results within the convergence definition.

2.4.3 Comparison with Observation

Another QA comparison is to see if the resulting overall inventory estimates correspond to environmental surveillance data and/or accepted literature estimates. This check serves as additional verification of the model performance. However, no comprehensive validation is currently possible because of the lack of independent field results for the sites in SIM. This comparison only incorporates data from where there is an accepted literature value in Diediker (1999) that was not determined to be in dispute with other historical information, for example, subject to correction for the presence of “less than” values in the reference literature.

For this comparison, a 99% estimate range of four analytes with reasonably comprehensive historical results (Cs-137, Sr-90, U-238, and Pu-239) was selected as the basis for comparison. Agreement is presumed between the model results and the accepted literature data if the literature result falls within the SIM estimated range. More sophisticated statistical tests are not warranted because the Diediker (1999) values do not have an agreed upon uncertainty definition.

Because of the lack of a comprehensive set of accepted reference values, there are no comparisons available for the tank leaks or most of the unplanned releases. Results for 179 of the 377 sites for each of the four specific analytes are provided in Section 6.0 at three different levels of resolution (zero-order, first order, and second order). The degree of agreement between model and observation for the selected sites and analytes is around 70%. The complete set of comparisons are presented and discussed in further detail in Section 6.0.

2.4.4 Latin Hypercube Sample Bin Size Evaluation

The convergence behavior of the simulation in a standard Monte Carlo scenario was found to be ill-behaved during the early testing of the OCB software (i.e., the simulation would not converge); therefore, SIM is operated using Latin hypercube sampling. A series of 25,000 run trials were performed using a varying number of results per bin to determine the most appropriate Latin hypercube parameter definition. SIM was run from the 50 bin case (500 results per bin) to the 1,000 bin case (25 results per bin). Theoretically, at least 33 results are necessary to satisfy the minimum amount of values required to provide legitimate means from each bin (e.g., extrapolating from the law of large numbers); however, a reasonable run-time for the model was also considered as a limitation. The selected modeling parameters (25,000 trials, 500 bins, 50 results per bin) appear to provide acceptable results and model run-times. The results from this series of tests provide confirmation that a reasonable selection of Latin hypercube parameters was used for the simulation.

2.4.5 Procedure Compliance

To comply with client QA protocols, spreadsheet verification and calculation verification was performed in accordance with CH2M HILL procedures to meet the requirements in the statement of work (CH2M HILL 2005a). These procedures dictate a series of inspections to be performed to verify the performance and integrity of the spreadsheets and calculations used. Additionally, a separate series of calculations using Crystal Ball was performed comparing the OCB results with those sites for the highest uncertainty sites (as measured by relative standard deviation [RSD]) to further confirm model convergence as well as provide calculation verification. These QA results are provided in Appendix B.

3.0 SIM DEVELOPMENT

This section describes the main assumptions and methods used to develop modeling inputs and relationships used in SIM Rev. 1. The data and methods used to develop these inputs are traceable, repeatable, and scalable. Each waste stream has different composition and degrees of uncertainty, related to the process chemistry and the timing of the radionuclide separation, influencing the modeling assumptions and data evaluation process. Additionally, each waste site may have a variety of waste streams that were disposed to it during the operating timeframe together with specific environmental conditions that need to be considered as well.

Data regarding waste sources, types, compositions, volumes, and locations for particular disposal sites were collected from multiple sources (Section 8.0, References). Numerous historical waste management and surveillance documents, reactor production information from ORIGEN2 (Watrous et al. 2002), and the HDW Model (Higley et al. 2004; Agnew et al. 1997a), and a number of engineering/technical assumptions were used to obtain waste stream composition, disposal volumes, uncertainty distributions, and other modeling parameters. Each of the parameter definition spreadsheets in the production workbook is a self-contained module that contains the comprehensive qualitative and quantitative descriptions necessary for executing the SIM calculations. These spreadsheets will be described in subsequent sections.

Section 3.1 describes the various assumptions, definitions, and boundary conditions used in the development of SIM. Section 3.2 describes the site selection process for the model. Section 3.3 describes the fundamentals of SIM (the equation and its components). Section 3.4 describes the uncertainty derivation and assignment process**.** Section 3.5 describes how the scalar correction factors applied to the inventory calculation were derived and applied in SIM.

3.1 MODEL ASSUMPTIONS, DEFINITIONS, AND BOUNDARY CONDITIONS

Numerous modeling assumptions, definitions, and boundary conditions are used in various capacities throughout SIM Rev. 1. These model elements are principally simplifications that enable the model to be reasonable in size and complexity and appropriately accommodate a wide variety of modeling situations; however, they are also used to extrapolate a variety of quantities in the absence of data and to provide guidance on how ambiguous situations with regard to data interpretation are addressed within SIM. This section provides fundamental background on the source information and assumptions used in developing SIM. These assumptions, definitions, and conditions are summarized in the following categories and are briefly discussed. Appendix A presents a more detailed discussion of the various assumptions and source information.

The SIM system includes the following definitions, assumptions, and boundary conditions:

- Assume that application of a minimum basis set of waste streams is appropriate and sufficient to describe disposal site inventories;

- Assume that waste management procedures and operating conditions are reasonably consistent throughout Hanford Site processes;
- Use or develop comprehensive waste stream compositions, such as HDW Rev. 5 waste stream definitions, where possible and maintain analyte correlations;
- Maintain simplicity in description of waste stream-waste site input allocations/ contributions, within known physical/chemical limits;
- Assume intrinsic contamination control measures and physical constraints generally prevented the loss of solids from the tank-canyon system; and
- Ensure that the waste stream compositions are as independent as practicable and minimize direct circularity in applying reference data values to modeling inputs.

The reference data integrity assumptions and boundary conditions are:

- Maintain alignment with available surveillance data with regard to waste stream-disposal site volume assignments and inventory values, where possible;
- Maintain alignment with Tank Farms regarding HDW stream compositions and chemistry assumptions, using contemporary sampling data sparingly;
- Enforce tank-canyon-disposal site mass balance assumption; and
- Use logical extensions of contemporary waste stream data for analogous (but data sparse) situations in the absence of early Hanford Site surveillance information.

The uncertainty development definitions, assumptions, and boundary conditions are:

- Assume that the campaign subdivisions for the ORIGEN2 reactor production data are appropriate groupings for defining uncertainty behavior;
- Assume that the various input variables are mathematically independent;
- Assume that the uncertainties defined for the radionuclide concentrations are well described by the ORIGEN2 beta distribution curve-fits (radionuclides) and that they are not substantially confounded by solubility behavior; and
- Assume that the inter-batch variability for a particular waste stream is encompassed by the selected uncertainty definition.

3.1.1 SIM System Definitions, Assumptions, and Boundary Conditions

A minimum set of waste streams is assumed to be a SIM modeling boundary condition. This assumption has a two-fold purpose: (1) it keeps the model from getting unwieldy in size and (2) forces critical evaluation of waste stream-disposal site environment. A model is not useful and does not explain much if there is no common behavior to exploit quantitatively and consistently to describe various observations. SIM disagreement with reference values and inconsistent behavior observed in SIM or the reference values between historically similar sites are cause for further investigation with respect to the model system bases and the reference data.

Processes represented in SIM are assumed to be well defined and Hanford Site personnel are assumed to have conducted waste management operations within control specifications, ensuring consistency in model treatment between geographically and chronologically separated disposal sites receiving similar wastes. Exceptions to this assumption were usually indicated from the available reference data and are dealt with explicitly or in other assumptions.

HDW Rev. 5 stream descriptions are used as a composition basis for disposal waste streams in most cases. The estimated HDW waste stream compositions (Agnew et al. 1997a; Higley et al. 2004) are assumed to be more representative of the waste conditions for liquid waste disposal sites at the time of disposal than contemporary tank sample data. This is assumed because the HDW Model waste stream compositions attempt to represent the waste compositions when the waste was produced, without the confounding effects of mixing, additional processing or changes as a function of time (other than radioactive decay).

The reference documents are often straightforward regarding the types and amounts of waste discharged to a site. This clarity is usually maintained when defining the waste types and volumes contributed to a site within SIM. Where the disposal site waste assignment or volume information is ambiguous, a simplified representation was developed. Generalized rules regarding the allocation of waste volumes, combining differently named waste streams with similar characteristics, and linearization of overall waste volume as a function of time have been established.

Very few waste streams disposed to the past-practice sites are considered to possess solids because of the waste management and surveillance practices employed during production operations and the general physical constraints of the system with regard to particulate entrainment (radiation monitors, settling tanks, no agitation, filtration, etc.). However, in certain instances, the surveillance data suggest that solids were present; thus, the presence of solids is allowed and inventory calculations incorporating solids are possible (on a site-year basis, ~6% of the inputs have solids; on a strict site basis, ~21% received solids). Thus, the default condition for SIM is not to incorporate entrained solids. But for certain waste streams and waste sites, the inclusion of entrained solids is reasonable from a physical and waste management operations perspective—laboratory wastes, decontamination waste, cold start wastes, and fuel fabrication wastes are all likely to have solids. In addition, selected process excursions where the conventional waste management practices were deemed inadequate to maintain containment are also considered as part of this evaluation (piping failures, overflow conditions, or poor settling).

Use of the HDW Model definitions for composition information partially addresses the difficulty of circularity with respect to the SIM inputs/output and use of/comparisons with the reference data in SIM Rev. 1. Because the HDW Model was developed in a manner far removed from SIM (even though they share some common references), the HDW Model is considered an independent source of composition information.

3.1.2 Reference Data Integrity Assumptions and Boundary Conditions

Extensive data from the various plant technical manuals, numerous process engineering memorandums, and surveillance data are used to derive and/or assign waste stream compositions, define waste site operations, and assign waste streams and associated volumes for a particular site. The references in Section 8.0 and Appendix A, Section A6.0, enumerate the various sources of technical and operational data used to establish and define the variables used to calculate inventories at the various waste sites. SIM maintains alignment with available data where appropriate. However, in certain instances, errors or discrepancies were observed in the inspection and evaluation of the data, and corrections (regarding waste stream assignment or waste volume) are introduced into the disposal site model definitions.

Very little contemporary sampling data (1989 to present) are used to develop waste stream descriptions or uncertainty definitions, and furthermore, no best-basis inventory data (CH2M HILL 2005b) are used to quantify disposal site inventories. However, sample data are used in SIM to quantify the solubility behavior of a variety of analytes more closely in the tank waste/disposal environment. This contemporary information is used to calibrate the solubility subroutine in the latest HDW Model (Higley et al. 2004). Because of the highly complex solubility environment in the process plants and in the waste tanks, this approach is considered an acceptable, practical compromise in modeling the system. In addition to being comprehensive in description, enforcing consistent solubility behavior, and minimizing circularity in SIM, the HDW Model waste streams have several desirable features: they are internally mass and charge balanced, the individual solubilities of the various analytes are specified (and can be modified as data dictates), radionuclides have been decayed to a common date (January 1, 2001), and the overall system inputs and outputs are mass balanced.

The mass balance boundary condition is another significant assumption, especially for the radionuclides. The impact of this assumption is that for purposes of comparison to reference data, the tank-canyon-disposal site system is considered “closed,” even though in actuality there are likely unquantified losses to the environment. The role of atmospheric releases for volatile analytes such as H-3 and I-129 can significantly impact soil inventory estimates if these losses can be better quantified and validated. Thus, whatever the initial, decayed, production values from ORIGEN2 are, the sum of the mean amounts in the tanks, canyons, and lost to the ground for purposes of evaluation must be equal to that initial production amount. These conditions assist in evaluating the results and help ensure that the soil inventory results maintain mass balance within the documented waste volumes disposed and analyte masses produced/used at the Hanford Site.

Where changes in reactor production behavior are observed to occur as a function of time (e.g., changes to fuel cladding, fuel element design changes, or reactor operating power), but the basic chemical process is unchanged, new uncertainties based on that change are derived and assigned to that waste stream, without changing the base waste composition. Additionally, in cases where later waste production conditions existed that could be assumed analogous to earlier Hanford processing conditions and the surveillance data were collected from these later data, these data are assumed to be suitable representations of those earlier process conditions and used in SIM.

3.1.3 Uncertainty Development Definitions, Assumptions, and Boundary Conditions

Process phasing and changes in operating philosophy are clearly evident as a function of time when reviewing the data for developing SIM inputs (e.g., the timing of production and introduction of different operating procedures affected the amounts of particular analytes sent to the ground). The ORIGEN2 production data are grouped together on the same basis as the HDW Model Rev. 5 separations. Thus, the SIM input structure is designed to reduce potential cross-contamination or "cross-talk" between processing regimes and aid in enforcing the overall and individual mass balance boundary conditions. This structure is dictated by how production and waste management operations were conducted at the Hanford Site—waste management practices segregated wastes in predictable ways, and the development and definition of the inputs mirrored those practices.

Because of the methods used to obtain the HDW concentration inputs, no further correlation corrections are imposed in SIM Rev. 1 and each parameter/analyte is considered to be an independent variable in the modeling calculations. This assumption is key in the mathematics of the Monte Carlo calculation.

The uncertainty definitions assigned from curve-fits of the ORIGEN2 production data often have substantial ranges, and these definitions are assumed to encompass the broad range of behavior observed for these analytes. However, the production variability is acknowledged to be potentially confounded with the chemical behavior (solubility) of the various species. The interaction of chemical behavior, thermodynamic properties, and the dynamic chemical conditions in the tanks results in very large uncertainties for most radioactive species in these waste streams. There are limited literature data on the behavior of these species under the waste stream/tank storage conditions (alkaline, with moderate to high-ionic strength, multi-component solutions) that could be used to define an independent set of uncertainty distributions. Furthermore, the Crystal Ball data-fitting treatment of the derived beta distributions could be considered the most conservative quantification interpretation for this distribution because the lower limit in this treatment always includes zero, resulting in broader uncertainties. Therefore, the derived beta distributions are considered appropriate uncertainty representations for these analytes.

The separation processes are assumed to have been operated within specifications and abrupt changes in waste stream compositions and/or uncertainties are represented by new waste streams. Although there is evidence of modest process evolution, most of these changes do not result in practical changes to waste composition during the selected campaign timeframe and the batch-to-batch variability is assumed to be encompassed by the assigned uncertainty. Thus, the waste streams are assumed to not change rapidly over time, and the mean waste stream analyte concentrations are present in fixed ratios (i.e., correlated) to each other within a particular uncertainty regime.

3.2 MODEL SITE SELECTION

There are several tasks associated with site selection for inclusion in SIM Rev. 1. The first task is to evaluate the Waste Information Data System (WIDS) to determine the sites that are appropriate to model using SIM. There are several thousand waste sites documented in WIDS (DOE-RL 2002), covering the entire Hanford Site. The initial constraint excludes solid waste sites from consideration. Another constraint confines the analysis to the 200 Area Plateau. However, as a result of client input, certain tank farm leak/UPR sites were added or eliminated because their status changed as a result of additional analysis, and a select number of sites from the 300 Area were added. As a result of this selection process and client direction, 377 sites can be currently modeled using SIM. Appendix A, Section A5.0 presents the sites simulated in SIM Rev. 1 and their grouping membership.

The total quantified volume for the selected liquid waste disposal sites is ~1,023,000 ML. The overall mean volume for the tank leaks is estimated at 2.18 ML, and for the various unplanned release sites, the loss volume is estimated to be 3,419 ML. For comparison, the underground storage tanks at the Hanford Site contain approximately 200 ML of waste.

3.2.1 Disposal Sites and Unplanned Releases

The principal source for total disposal volume, waste stream assignment, and site location information is the Waste Information Data System (WIDS) database (DOE-RL 2002). This information is corroborated (and modified or corrected in some cases) from several other references and source documents cited in Section 8.0, and in certain instances, where there was no volume information available, engineering volume estimates and waste stream assignments were prepared. Maxfield (1979) also provided information of a more limited nature for waste types and waste stream composition.

3.2.2 Tank and Ancillary Equipment Leaks

Field and Jones (2005) is used as the principal source of data to define the date and volume of the tank and ancillary equipment leaks using the HDW Model Rev. 5. In SIM Rev. 1, the tank farm leaks are modeled as a small number of individually contributing components to the total leak volume using the fractional proportion of the various waste streams present in the tank during the leak timeframe. Once the date and volume of the leak event are established, the HDW Model is run for each source tank up to the date for each event. The tank leak descriptions result from the supernatant mixing model (SMM) assumptions of ideal mixing. The tank “memory” of all of the waste that passed through it (except for sluiced tanks, whose history is reset) and any solubility modifications that may be indicated from other data result in a specific tank composition for that date. These compositions are linear combinations of the different waste streams contributing to the inventory of a tank; thus, the estimated liquid composition of the tank when it was considered to have leaked is used. The basis for the selected tank leak compositions is further explained in Section 3.3.2 and Appendix A. No solids are considered lost in the case of a tank leak because of an assumed filtering effect.

3.3 MODEL PARAMETER DEFINITION

SIM is executing a basic equation that computes the mass or activity of a particular constituent. The general form of this equation is:

$I = \rho * C * V$ (Equation 3.1);

Inventory = density*concentration*volume

Because in some cases there are entrained solids included as part of the overall inventory, both phases of a waste stream must be computed, resulting in a slightly more complicated version of the equation:

$I = \rho_l * C_l * V_t * (1 - V_{\%s}) + \rho_s * C_s * V_{\%s}$ (Equation 3.2);

Inventory = density (liquid)*concentration (liquid)*total volume*(1-volume percent solids) + density (solids)*concentration (solids)*volume percent solids.

This form of the equation was selected based on the observed prevalence of the units associated with the analytical data, and these parameters are also presented in the HDW Model waste stream descriptions. The following sections will describe each of these parameters in more detail.

3.3.1 Density

The physical and chemical assumptions regarding density were not considered to substantially impact the results for inventory or uncertainty in SIM. Using a bulk density for both phases appears to be a reasonable representation of the stream condition, and the bulk density of the waste components does not appear to be confounded by the presence of gas as can happen in the tanks. The HDW waste stream densities used in the calculation are considered reasonable descriptions of the waste under the disposal conditions. Surveillance documentation often had density measurements as part of the overall data, and these values were used for calculating inventory based on non-HDW waste streams. Furthermore, the lower bounding values for both the aqueous and non-aqueous phase liquids that are not based on the HDW Model correspond to observed/reference values.

The minimum density for an aqueous stream was constrained to be no less than ~0.97 g/mL, and the maximum density was constrained to be no larger than ~2.1 g/mL. The solids densities are taken from the HDW Model directly and on a bulk basis have a similarly narrow range observed in tank farm samples. The bounding values for the various solids are within the observed tank sample data ranges (~1.05-2.1 g/mL).

3.3.2 Waste Stream Composition (Concentration)

Except as noted in Table 3-1, the HDW Model (Agnew et al. 1997a; Higley et al. 2004) waste stream values are used (and modified when appropriate) for input composition and uncertainty information. The liquid waste disposal sites and unplanned releases each used the same set of waste streams. The number of waste streams available in SIM has also increased in the latest version, from 16 to 196 waste streams. Table 3-1 presents the waste streams that are currently used and available in SIM. The waste stream label provides information regarding its chemical process origin and the uncertainty associated with the accompanying radionuclides. This list includes the newly derived HDW Rev. 5 waste stream descriptions, other sources used as a basis for waste stream composition, and incorporates the appropriate changes in uncertainties for waste streams that were produced over a long period of time. The referenced waste stream values and general derivation descriptions for each waste stream are presented in Appendix A. Specific information regarding waste stream derivation is included as part of the waste stream workbook in Appendix D.

Table 3-1. Soil Inventory Model Waste Streams and Source Information. (6 Sheets)

SIM Waste Stream Label	Reference Information
1C Evap (BT2)	HDW Rev. 5 (Higley et al. 2004)
1C1 (BT1)	HDW Rev. 5 (Higley et al. 2004)
1C2 (BT2)	HDW Rev. 5 (Higley et al. 2004)
1CFeCN (BT2)	HDW Rev. 5 (Higley et al. 2004)
209-E Reflector Wtr (BT1)	WHC-EP-0342 Addendum (Add.) 31 (WHC 1990o)
209-E Reflector Wtr (BT2)	WHC-EP-0342 Add. 31 (WHC 1990o)
209-E Reflector Wtr (P1)	WHC-EP-0342 Add. 31 (WHC 1990o)
209-E Reflector Wtr (P2)	WHC-EP-0342 Add. 31 (WHC 1990o)
209-E Reflector Wtr (P2')	WHC-EP-0342 Add. 31 (WHC 1990o)
209-E Reflector Wtr (P3)	WHC-EP-0342 Add. 31 (WHC 1990o)
222-S Lab Wst (P1)	WHC-EP-0342 Add. 9 (WHC 1990d) and Add. 13 (WHC 1990g) w/scaling factors
222-S Lab Wst (P2)	WHC-EP-0342 Add. 9 (WHC 1990d) and Add. 13 (WHC 1990g) w/scaling factors
222-S Lab Wst (P2')	WHC-EP-0342 Add. 9 (WHC 1990d) and Add. 13 (WHC 1990g) w/scaling factors
222-S Lab Wst (P3)	WHC-EP-0342 Add. 9 (WHC 1990d) and Add. 13 (WHC 1990g) w/scaling factors
222-S Lab Wst Wtr (P2)	WHC-EP-0342 Add. 13 (WHC 1990g) and Add. 10 (WHC 1990e)
222-S Lab Wst Wtr (P2')	WHC-EP-0342 Add. 13 (WHC 1990g) and Add. 10 (WHC 1990e)
222-S Lab Wst Wtr (P3)	WHC-EP-0342 Add. 13 (WHC 1990g) and Add. 10 (WHC 1990e)
222-S Lab Wst Wtr (R1)	WHC-EP-0342 Add. 13 (WHC 1990g) and Add. 10 (WHC 1990e)
222-S Lab Wst Wtr (R2)	WHC-EP-0342 Add. 13 (WHC 1990g) and Add. 10 (WHC 1990e)
224 (BT1)	HDW Rev. 5 (Higley et al. 2004)
224 (BT2)	HDW Rev. 5 (Higley et al. 2004)
231-Z Metal Lab (Z2)	Barrington (1990); HNF-1989 Rev. 1 (Jones 1998); DOE/RL-91-58 (DOE-RL 1992b); HNF-1744 (Diediker 1999)
232-Z Inc (Z1)	Barrington (1990); HNF-1989 Rev. 1 (Jones 1998); HNF-1744 (Diediker 1999)
232-Z Inc (Z2)	Barrington (1990); HNF-1989 Rev. 1 (Jones 1998); HNF-1744 (Diediker 1999)

Table 3-1. Soil Inventory Model Waste Streams and Source Information. (6 Sheets)

SIM Waste Stream Label	Reference Information
234-5Z (BT1) D-6	HNF-1744 (Diediker 1999); WHC-EP-0342 Add. 8 (WHC 1990c)
234-5Z (Z1) D-6	HNF-1744 (Diediker 1999); WHC-EP-0342 Add. 8 (WHC 1990c)
234-5Z (Z2) D-6	HNF-1744 (Diediker 1999); WHC-EP-0342 Add. 8 (WHC 1990c)
242-A Cond (P2')	WHC-EP-0342 Add. 26 (WHC 1990m)
242-A Cond (P3)	WHC-EP-0342 Add. 26 (WHC 1990m)
242-A Cond_CT (P3)	WHC-EP-0342 Add. 26 (WHC 1990m)
242-B (BT2) Evap Cond	WHC-EP-0342 Add. 17 (WHC 1990h)
242-S Evap Cond (R2)	WHC-EP-0342 Add. 29 (WHC 1990n)
242-T Evap Cond (R2)	WHC-EP-0342 Add. 17 (WHC 1990h)
242-T Evap Cond (Z2)	WHC-EP-0342 Add. 29 (WHC 1990n) w/misc. derivation
242-Z Am Rec (Z2)	Barrington (1990); HNF-1989 Rev. 1 (Jones 1998); Mercer (1986); HNF-1744 (Diediker 1999)
2C1 (BT1)	HDW Rev. 5 (Higley et al. 2004)
2C2 (BT2)	HDW Rev. 5 (Higley et al. 2004)
300 CW (Z1)	Mercer (1986) w/HDW Rev. 5 (Higley et al. 2004)
300 CW (Z2)	Mercer (1986) w/HDW Rev. 5 (Higley et al. 2004)
5-6 (BT1)	HDW Rev. 5 (Higley et al. 2004) with assumed dilution
5-6 (BT2)	HDW Rev. 5 (Higley et al. 2004) with assumed dilution
A1-SltCk(Z2)	HDW Rev. 5 (Higley et al. 2004)
A2-SltSlr(Z2)	Unused--HDW Rev. 5 (Higley et al. 2004)
BiPO4 (BT1) Chem Sewer	Derived from HDW Rev. 5 sources (Higley et al. 2004)
BiPO4 (BT1) Cool Wtr-Stm Cond	Derived from HDW Rev. 5 sources (Higley et al. 2004)
BiPO4 (BT1) Stack Drain	Derived from HDW Rev. 5 sources (Higley et al. 2004)
BiPO4 (BT2) Chem Sewer	Derived from HDW Rev. 5 sources (Higley et al. 2004)
BiPO4 (BT2) Cool Wtr-Stm Cond	Derived from HDW Rev. 5 sources (Higley et al. 2004)
BiPO4 (BT2) Stack Drain	Derived from HDW Rev. 5 sources (Higley et al. 2004)
BYSLT (BT2)	HDW Rev. 5 (Higley et al. 2004)
CEM(NA)	Unused--HDW Rev. 5 (Higley et al. 2004)
Conc Misc UNH Streams (P1)	WHC-EP-0342 Add. 19 (WHC 1990i) and HDW Rev. 5 assumption
Conc Misc UNH Streams (P2)	WHC-EP-0342 Add. 19 (WHC 1990i) and HDW Rev. 5 assumption
Conc Misc UNH Streams (P2')	WHC-EP-0342 Add. 19 (WHC 1990i) and HDW Rev. 5 assumption
Conc Misc UNH Streams (P3)	WHC-EP-0342 Add. 19 (WHC 1990i) and HDW Rev. 5 assumption
Conc Misc UNH Streams (R1)	WHC-EP-0342 Add. 19 (WHC 1990i) and HDW Rev. 5 assumption
Conc Misc UNH Streams (R2)	WHC-EP-0342 Add. 19 (WHC 1990i) and HDW Rev. 5 assumption
CWP1 (CWP1)	HDW Rev. 5 (Higley et al. 2004)
CWP2 (CWP2)	HDW Rev. 5 (Higley et al. 2004)
CWR1 (CWR1)	HDW Rev. 5 (Higley et al. 2004)
CWR2 (CWR2)	HDW Rev. 5 (Higley et al. 2004)
CWZr1 (CWZr1)	HDW Rev. 5 (Higley et al. 2004)
CWZr2 (CWZr2)	Unused--HDW Rev. 5 (Higley et al. 2004)
DE(NA)	Unused--HDW Rev. 5 (Higley et al. 2004)
Decon Stack Drain (BT2)	Derived from HDW Rev. 5 sources (Higley et al. 2004)
Decon Stack Drain (R2)	Derived from HDW Rev. 5 sources (Higley et al. 2004)
Decon Wst (BT1)	Derived from HDW Rev. 5 sources (Higley et al. 2004)
Decon Wst (BT2)	Derived from HDW Rev. 5 sources (Higley et al. 2004)
Decon Wst (P1)	Derived from HDW Rev. 5 sources (Higley et al. 2004)
Decon Wst (P2)	Derived from HDW Rev. 5 sources (Higley et al. 2004)
Decon Wst (P2')	Derived from HDW Rev. 5 sources (Higley et al. 2004)
Decon Wst (P3)	Derived from HDW Rev. 5 sources (Higley et al. 2004)
Decon Wst (R1)	Defunct
Decon Wst (R2)	Derived from HDW Rev. 5 sources (Higley et al. 2004)

Table 3-1. Soil Inventory Model Waste Streams and Source Information. (6 Sheets)

SIM Waste Stream Label	Reference Information
Dil Misc UNH Streams (BT2)	WHC-EP-0342 Add. 19 (WHC 1990i)
Dil Misc UNH Streams (P1)	WHC-EP-0342 Add. 19 (WHC 1990i)
Dil Misc UNH Streams (P2)	WHC-EP-0342 Add. 19 (WHC 1990i)
Dil Misc UNH Streams (P2')	WHC-EP-0342 Add. 19 (WHC 1990i)
Dil Misc UNH Streams (P3)	WHC-EP-0342 Add. 19 (WHC 1990i)
Dil Misc UNH Streams (R1)	WHC-EP-0342 Add. 19 (WHC 1990i)
Dil Misc UNH Streams (R2)	WHC-EP-0342 Add. 19 (WHC 1990i)
ITS Cool Wtr-Cond (BT2)	Derived using average of 242-B and 242-S Condensates
Laundry Wst Wtr (BT1)	WHC-EP-0141-1 (Coony and Thomas 1989); WHC-EP-0141-2 (Brown et al. 1990); WHC-EP-0527 (WHC 1992a, 1992b, 1993, 1994, 1995, and 1996; Gleckler 1997, 1998); RHO-HS-SR-81-3 to RHO-HS-SR-86-3 4Q LIQ (Aldrich 1985, 1986, and 1987; Sliger 1982 and 1983)
Laundry Wst Wtr (BT2)	WHC-EP-0141-1 (Coony and Thomas 1989); WHC-EP-0141-2 (Brown et al. 1990); WHC-EP-0527 (WHC 1992a, 1992b, 1993, 1994, 1995, and 1996; Gleckler 1997, 1998); RHO-HS-SR-81-3 to RHO-HS-SR-86-3 4Q LIQ (Aldrich 1985, 1986, and 1987a; Sliger 1982 and 1983)
Laundry Wst Wtr (P2')	WHC-EP-0141-1 (Coony and Thomas 1989); WHC-EP-0141-2 (Brown et al. 1990); WHC-EP-0527 (WHC 1992a, 1992b, 1993, 1994, 1995, and 1996; Gleckler 1997, 1998); RHO-HS-SR-81-3 to RHO-HS-SR-86-3 4Q LIQ (Aldrich 1985, 1986, and 1987a; Sliger 1982 and 1983)
Laundry Wst Wtr (P3)	WHC-EP-0141-1 (Coony and Thomas 1989); WHC-EP-0141-2 (Brown et al. 1990); WHC-EP-0527 (WHC 1992a, 1992b, 1993, 1994, 1995, and 1996; Gleckler 1997, 1998); RHO-HS-SR-81-3 to RHO-HS-SR-86-3 4Q LIQ (Aldrich 1985, 1986, and 1987a; Sliger 1982 and 1983)
Laundry Wst Wtr (R2)	WHC-EP-0141-1(Coony and Thomas 1989) ; WHC-EP-0141-2 (Brown et al. 1990); WHC-EP-0527 (WHC 1992a, 1992b, 1993, 1994, 1995, and 1996; Gleckler 1997, 1998); RHO-HS-SR-81-3 to RHO-HS-SR-86-3 4Q LIQ (Aldrich 1985, 1986, and 1987a; Sliger 1982 and 1983)
MW1 (BT1)	HDW Rev. 5 (Higley et al. 2004)
MW2 (BT2)	HDW Rev. 5 (Higley et al. 2004)
N Decon Wst (P2)	Derived from HDW Rev. 5 sources (Higley et al. 2004)
NIT(NA)	Unused--HDW Rev. 5 (Higley et al. 2004)
OrgSltCk(P2')	Defunct
P3AZ1(P3)	Unused--HDW Rev. 5 (Higley et al. 2004)
P3AZ2(P3)	Unused--HDW Rev. 5 (Higley et al. 2004)
PASF (P2)	HDW Rev. 5 (Higley et al. 2004); HNF-1744 (Diediker 1999)
PASF (P2')	HDW Rev. 5 (Higley et al. 2004); ARH-1972 (Hanson 1971); HNF-1744 (Diediker 1999)
PASF (P3)	HDW Rev. 5 (Higley et al. 2004); ARH-1972 (Hanson 1971); HNF-1744 (Diediker 1999)
PFeCN1 (BT1)	HDW Rev. 5 (Higley et al. 2004)
PFeCN2 (BT2)	HDW Rev. 5 (Higley et al. 2004)
Powerhouse Wst Wtr (NA)	WHC-SD-LEF-RPT-001 Rev. 0 (Lueck 1995)
PUREX (all) Stack Drain WC	Reference Working Sheet - Waste Stream Workbook (WSWB); Appendix D
PUREX (P1) Chem Sewer	WHC-EP-0342 Add. 2 (WHC 1990a) scaled to timeframe
PUREX (P1) Cold Start	HDW Rev. 5 (Higley et al. 2004)

Table 3-1. Soil Inventory Model Waste Streams and Source Information. (6 Sheets)

SIM Waste Stream Label	Reference Information
PUREX (P1) Cool Wtr-Stm Cond	WHC-EP-0342 Add. 20 (WHC 1990j) and 216-A-25 data (Diediker 1999; DOE/RL-92-05 [DOE-RL 1993]; and RHO-HS-SR-84-3 4Q LIQ [Aldrich 1985])
PUREX (P1) Org Wst	HDW Rev. 5 (Higley et al. 2004); HW-31000-DEL (GE 1955)
PUREX (P1) Org Wst aqu_OWW1	HDW Rev. 5 (Higley et al. 2004)
PUREX (P1) Org Wst aqu_OWW2	HDW Rev. 5 (Higley et al. 2004)
PUREX (P1) Stack Drain	Derived from HDW Rev. 5 sources (Higley et al. 2004)
PUREX (P1) Tank Farm Cond	WHC-EP-0342 Add. 26 (WHC 1990m)
PUREX (P2) Chem Sewer	WHC-EP-0342 Add. 2 (WHC 1990a) scaled to timeframe
PUREX (P2') Chem Sewer	WHC-EP-0342 Add. 2 (WHC 1990a) scaled to timeframe
PUREX (P2) Cool Wtr-Stm Cond	WHC-EP-0342 Add. 20 (WHC 1990j) and 216-A-25 data (Diediker 1999; DOE/RL-92-05 [DOE-RL 1993]; and RHO-HS-SR-84-3 4Q LIQ [Aldrich 1985])
PUREX (P2') Cool Wtr-Stm Cond	WHC-EP-0342 Add. 20 (WHC 1990j) and 216-A-25 data (Diediker 1999; DOE/RL-92-05 [DOE-RL 1993]; and RHO-HS-SR-84-3 4Q LIQ [Aldrich 1985])
PUREX (P2) Org Wst	HDW Rev. 5 (Higley et al. 2004); HW-31000-DEL (GE 1955)
PUREX (P2') Org Wst	HDW Rev. 5 (Higley et al. 2004); HW-31000-DEL (GE 1955)
PUREX (P2) Org Wst aqu_OWW1	HDW Rev. 5 (Higley et al. 2004)
PUREX (P2) Org Wst aqu_OWW2	HDW Rev. 5 (Higley et al. 2004)
PUREX (P2') Org Wst aqu_OWW3	HDW Rev. 5 (Higley et al. 2004)
PUREX (P2) Stack Drain	Derived from HDW Rev. 5 sources (Higley et al. 2004)
PUREX (P2') Stack Drain	Derived from HDW Rev. 5 sources (Higley et al. 2004)
PUREX (P2) Tank Farm Cond	WHC-EP-0342 Add. 23 (WHC 1990l)
PUREX (P2') Tank Farm Cond	WHC-EP-0342 Add. 23 (WHC 1990l)
PUREX (P3) Chem Sewer	WHC-EP-0342 Add. 2 (WHC 1990a)
PUREX (P3) Cool Wtr-Stm Cond	WHC-EP-0342 Add. 20 (WHC 1990j) and 216-A-25 data (Diediker 1999; DOE/RL-92-05 [DOE-RL 1993]; and RHO-HS-SR-84-3 4Q LIQ [Aldrich 1985])
PUREX (P3) Process Cond	WHC-EP-0342 Add. 12 (WHC 1990f)
PUREX (P3) Stack Drain	Derived from HDW Rev. 5 sources (Higley et al. 2004)
PUREX (P3) Tank Farm Cond	WHC-EP-0342 Add. 23 (WHC 1990l)
PUREX P1 (P1)	HDW Rev. 5 (Higley et al. 2004)
PUREX P2 (P2)	HDW Rev. 5 (Higley et al. 2004)
PUREX P2' (P2')	Unused--HDW Rev. 5 (Higley et al. 2004)
PUREX P3 (P3)	Defunct
PUREX PL1 (P1)	HDW Rev. 5 (Higley et al. 2004)
PUREX PL2 (P3)	Unused--HDW Rev. 5 (Higley et al. 2004)
R1 (R1)	HDW Rev. 5 (Higley et al. 2004)
R2 (R2)	HDW Rev. 5 (Higley et al. 2004)
Recuplex (BT1) aqu	Barrington (1990); HNF-1989 Rev. 1 (Jones 1998); Mercer (1986); HNF-1744 (Diediker 1999)
Recuplex (BT1) org.	Barrington (1990); HNF-1989 Rev. 1 (Jones 1998); Mercer (1986); HNF-1744 (Diediker 1999)
Recuplex (Z1) aqu	Barrington (1990); HNF-1989 Rev. 1 (Jones 1998); Mercer (1986); HNF-1744 (Diediker 1999)
Recuplex (Z1) org.	Barrington (1990); HNF-1989 Rev. 1 (Jones 1998); Mercer (1986); HNF-1744 (Diediker 1999)
Recuplex (Z2) aqu	Barrington (1990); HNF-1989 Rev. 1 (Jones 1998); Mercer (1986); HNF-1744 (Diediker 1999)
Recuplex (Z2) org.	Barrington (1990); HNF-1989 Rev. 1 (Jones 1998); Mercer (1986); HNF-1744 (Diediker 1999)

Table 3-1. Soil Inventory Model Waste Streams and Source Information. (6 Sheets)

SIM Waste Stream Label	Reference Information
REDOX (P2') Cool Wtr	Derived from HDW Rev. 5 sources (Higley et al. 2004)
REDOX (P2') Stack Drain	Derived from HDW Rev. 5 sources (Higley et al. 2004)
REDOX (P2') Tank Farm Cond	WHC-EP-0342 Add. 26 (WHC 1990m)
REDOX (P3) Stack Drain	Derived from HDW Rev. 5 sources (Higley et al. 2004)
REDOX (R1) Chem Sewer	Defunct
REDOX (R1) Cool Wtr	Derived from HDW Rev. 5 sources (Higley et al. 2004)
REDOX (R1) Org	Derived from HDW Rev. 5 sources (Higley et al. 2004); HW-18700 (GE 1951b)
REDOX (R1) Tank Farm Cond	WHC-EP-0342 Add. 29 (WHC 1990n)
REDOX (R2) Chem Sewer	Defunct
REDOX (R2) Cool Wtr	Derived from HDW Rev. 5 sources (Higley et al. 2004)
REDOX (R2) Org	Derived from HDW Rev. 5 sources (Higley et al. 2004); HW-18700 (GE 1951b)
REDOX (R2) Tank Farm Cond	WHC-EP-0342 Add. 29 (WHC 1990n)
REDOX Cold Start (R1)	Derived from HDW Rev. 5 sources (Higley et al. 2004)
REDOX Cold Start (R1) Org	Derived from HDW Rev. 5 sources (Higley et al. 2004); HW-18700 (GE 1951b)
REDOX D-1 (R1)	HW-59359 (Baldridge 1959); HW-60115 (GE 1959); DOE/RL-91-60 (DOE-RL 1992c); HNF-1744 (Diediker 1999); RHO-CD-673 (Maxfield 1979)
REDOX D-1 (R2)	HW-59359 (Baldridge 1959); HW-60115 (GE 1959); DOE/RL-91-60 (DOE-RL 1992c); HNF-1744 (Diediker 1999); RHO-CD-673 (Maxfield 1979)
REDOX D-2 (R1)	HW-59359 (Baldridge 1959); HW-60115 (GE 1959); DOE/RL-91-60 (DOE-RL 1992c); HNF-1744 (Diediker 1999); RHO-CD-673 (Maxfield 1979)
REDOX D-2 (R2)	HW-59359 (Baldridge 1959) ; HW-60115; (GE 1959) DOE/RL-91-60 (DOE-RL 1992c); HNF-1744 (Diediker 1999); RHO-CD-673 (Maxfield 1979)
REDOX Stack Drain (R1)	Derived from HDW Rev. 5 sources (Higley et al. 2004)
REDOX Stack Drain (R2)	Derived from HDW Rev. 5 sources (Higley et al. 2004)
RG Process (BT1)	Barrington (1990); HNF-1989 Rev. 1 (Jones 1998); HNF-1744 (Diediker 1999)
RG Process (Z1)	Defunct
RG Process (Z2)	Defunct
RSLT (R2)	HDW Rev. 5 (Higley et al. 2004)
S1-SltCk(P2')	HDW Rev. 5 (Higley et al. 2004)
S2-SltSlr(P2')	HDW Rev. 5 (Higley et al. 2004)
Salt Slurry(P2')	Unused--HDW Rev. 5 (Higley et al. 2004)
Spent Nitric Acid (BT2)	HW-31000-DEL (GE 1955) w/ misc derivation
Spent Nitric Acid (P1)	HW-31000-DEL (GE 1955)
Spent Nitric Acid (P2)	HW-31000-DEL (GE 1955)
Spent Nitric Acid (P2')	HW-31000-DEL (GE 1955)
Spent Nitric Acid (P3)	HW-31000-DEL (GE 1955)
Spent Nitric Acid (R1)	HW-31000-DEL (GE 1955) w/ misc derivation
Spent Nitric Acid (R2)	HW-31000-DEL (GE 1955) w/ misc derivation
Sr-Cs Rec (P1) Cool Wtr	WHC-EP-0342 Add. 22 (WHC 1990k)
Sr-Cs Rec (P1) Stack Drain	WHC-EP-0342 Add. 17(WHC 1990h); w/ misc. derivation
Sr-Cs Rec (P2') Chem Sewer	WHC-EP-0342 Add. 6 (WHC 1990b)
Sr-Cs Rec (P2) Cool Wtr	WHC-EP-0342 Add. 22 (WHC 1990k)
Sr-Cs Rec (P2') Cool Wtr	WHC-EP-0342 Add. 22 (WHC 1990k)
Sr-Cs Rec (P2) Stack Drain	WHC-EP-0342 Add. 17(WHC 1990h); w/ misc. derivation

Table 3-1. Soil Inventory Model Waste Streams and Source Information. (6 Sheets)

SIM Waste Stream Label	Reference Information
Sr-Cs Rec (P2') Stack Drain	WHC-EP-0342 Add. 17 (WHC 1990h); w/ misc. derivation
Sr-Cs Rec (P3) Chem Sewer	WHC-EP-0342 Add. 6 (WHC 1990b)
Sr-Cs Rec (P3) Cool Wtr	WHC-EP-0342 Add. 22 (WHC 1990k)
Sr-Cs Rec (P3) Stack Drain	WHC-EP-0342 Add. 17 (WHC 1990h); w/ misc. derivation
Sr-Cs Rec (R1) Chem Sewer	WHC-EP-0342 Add. 6 (WHC 1990b)
Sr-Cs Rec (R1) Cool Wtr	WHC-EP-0342 Add. 22 (WHC 1990k)
Sr-Cs Rec (R2) Chem Sewer	WHC-EP-0342 Add. 6 (WHC 1990b)
Sr-Cs Rec Org Wst (P2)_B	HDW Rev. 5 (Higley et al. 2004)
Sr-Cs Rec Org Wst (P2')_CSR	HDW Rev. 5 (Higley et al. 2004)
Sr-Cs Rec Org Wst aqu (P2)_BL	HDW Rev. 5 (Higley et al. 2004)
Sr-Cs Rec Org Wst aqu(P2')_AR	HDW Rev. 5 (Higley et al. 2004)
Sr-Cs Rec Wst (P1)_HS	HDW Rev. 5 (Higley et al. 2004)
Sr-Cs Rec Wst (P2)_SRR	HDW Rev. 5 (Higley et al. 2004)
T2-SltCk(P2')	HDW Rev. 5 (Higley et al. 2004)
TBP-UR (BT2)	HDW Rev. 5 (Higley et al. 2004)
TBP-UR Org Wst (BT2)	HDW Rev.5 and HW-19140 (GE 1951a) w/ derivation information
TFeCN (BT2)	HDW Rev. 5 (Higley et al. 2004)
TH1 (TH2)	HDW Rev. 5 (Higley et al. 2004)
TH2 (TH2)	HDW Rev. 5 (Higley et al. 2004)
Z Complex Chem Sewer (NA)	Rodgers (1986); Abramowski (1985)
Z Complex Chem Sewer_NCT (NA)	Rodgers (1986); Abramowski (1985)
Z Complex Cool Wtr-Cond (BT1)	WHC-EP-0342 Add. 8 (WHC 1990c)
Z Complex Cool Wtr-Cond (Z1)	WHC-EP-0342 Add. 8 (WHC 1990c)
Z Complex Cool Wtr-Cond (Z2)	WHC-EP-0342 Add. 8 (WHC 1990c)
Z Complex Lab Wst (BT1)	Barrington (1990); HNF-1989 Rev. 1 (Jones 1998); HNF-1744 (Diediker 1999)
Z Complex Lab Wst (Z1)	Barrington (1990); HNF-1989 Rev. 1 (Jones 1998); HNF-1744 (Diediker 1999)
Z Complex Lab Wst (Z2)	Barrington (1990); HNF-1989 Rev. 1 (Jones 1998); HNF-1744 (Diediker 1999)
Z Complex Stack Drain (BT1)	Assumed 1.1 dilution of Z Complex cooling water
Z Complex Stack Drain (Z1)	Assumed 1.1 dilution of Z Complex cooling water
Z Complex Stack Drain (Z2)	Assumed 1.1 dilution of Z Complex cooling water
Z Complex Stack Drain_NCT (Z2)	Assumed 1.1 dilution of Z Complex cooling water
Z(Z2)	HDW Rev. 5 (Higley et al. 2004)

Determining the composition of a tank farm leak requires several steps, because in general a tank has processed numerous waste streams as a function of waste management activities that were ongoing at the Hanford Site, and leaks are rarely the result of the loss of one waste stream exclusively. Using the HDW Model together with the supernatant mixing model (SMM) subroutine, a transaction history for a tank can be run to any particular point in time and a composition of the tank ascertained. Once this composition has been set, the leak volume can be used to compute an inventory. The HDW Model Rev. 5 (Higley et al. 2004) waste stream compositions and SIM inventory calculations were applied to leak dates and volumes established in Field and Jones (2005).

In certain instances, process knowledge regarding the condition of the tank is used to override or modify the SMM definition (e.g., boiling tanks in SX) because that tank feature meant that using the unmodified SMM description for the tank leak inventory would not appropriately represent the leak composition in SIM. Dates and volumes of the tank leaks used in SIM are derived principally using Field and Jones (2005). They used combination of specific technical documentation, tank surveillance data, spectral gamma logging data, and historical transaction data evaluate and quantify the date and volume associated with each leak. These data formed the basis to determine whether a previously documented tank leak event was included for simulation. Where a discrepancy between SIM interpretations of the event data diverges from the convention used by Tank Farms (reported in Field and Jones [2005]), these differences are noted. Accordingly, Field and Jones (2005) conclude that only 50 of the 68 leak events occurred, and only those 50 are evaluated using SIM. Table 3-2 relates the tank farm leak events and the description of their derivation.

Table 3-2. Tank Farm Leak Event Sites and Definitions. (3 Sheets)

Tank	Volume (gal)	Year	Site Description
241-A-103	5500	1987	Zero Solids. Unadjusted SMM definition for tank leak date of 1987.
241-A-104	2000	1975	Zero Solids. Unadjusted SMM definition for tank leak date of 1975.
241-A-105	1000	1965	Zero Solids. Unadjusted SMM definition for tank leak date of 1965, plus subsequent cooling water addition.
241-AX-102	3000	1975	Zero Solids. Unadjusted SMM definition for tank leak date of 1975.
241-B-107	14000	1965	Zero Solids. Unadjusted SMM definition for tank leak date of 1965.
241-B-110	10000	1969	Zero Solids. Unadjusted SMM definition for tank leak date of 1969.
241-B-112	2000	1972	Zero Solids. Unadjusted SMM definition for tank leak date of 1972.
241-B-201	1200	1965	Zero Solids. Unadjusted SMM definition for tank leak date of 1965.
241-B-203	300	1965	Zero Solids. Unadjusted SMM definition for tank leak date of 1965.
241-B-204	400	1965	Zero Solids. Unadjusted SMM definition for tank leak date of 1965.
241-BX-101	4000	1972	Zero Solids. Unadjusted SMM definition for tank leak date of 1972.
241-BX-102	91600	1951	Included Solids. Unadjusted SMM definition for tank leak date of 1951. MW1 solids are added to this overfill loss to reach estimated uranium values matching the historical descriptions of event.
241-BX-108	2500	1972	Zero Solids. Unadjusted SMM definition for tank leak date of 1972.
241-BY-103[1]	400	1973	Zero Solids. Adjusted SMM definition for tank leak date of 1973 to reflect ITS concentration of waste into BYSLT.
241-BY-107[1]	1200	1974	Zero Solids. Adjusted SMM definition for tank leak date of 1974 to reflect ITS concentration of waste into BYSLT.
241-BY-108[1]	400	1972	Zero Solids. Adjusted SMM definition for tank leak date of 1972 to reflect ITS concentration of waste into BYSLT.
241-C-101	1000	1968	Zero Solids. Unadjusted SMM definition for tank leak date of 1968.
241-C-105	1000	1972	Zero Solids. Unadjusted SMM definition for tank leak date of 1972.
241-C-110	2000	1969	Zero Solids. Unadjusted SMM definition for tank leak date of 1969.

Table 3-2. Tank Farm Leak Event Sites and Definitions. (3 Sheets)

Tank	Volume (gal)	Year	Site Description
241-C-111	5500	1968	Zero Solids. Unadjusted SMM definition for tank leak date of 1968.
241-C-201	550	1965	Zero Solids. Unadjusted SMM definition for tank leak date of 1965.
241-C-202	450	1965	Zero Solids. Unadjusted SMM definition for tank leak date of 1965.
241-C-203	400	1957	Zero Solids. Unadjusted SMM definition for tank leak date of 1957.
241-C-204	350	1957	Zero Solids. Unadjusted SMM definition for tank leak date of 1957.
241-S-104	24000	1965	Zero Solids. Adjusted SMM definition to this tank. SMM ideal mixing rules do not apply to this CWR2 overfill event because of the manner in which wastes were added.
241-SX-104	6000	1988	Zero Solids. Unadjusted SMM definition for tank leak date of 1988.
241-SX-107	15000	1963	Zero Solids. Adjusted 1963 SMM definition because of tank self-concentration effect. Used RSLT (R2) in SX tanks where the supernatant volume (Sup Vol) is less than half of the SMM volume (e.g., unconcentrated, original waste volume).
241-SX-108	35000	1966	Zero Solids. Adjusted 1966 SMM definition because of tank self-concentration effect. Used RSLT (R2) in SX tanks where the supernatant volume (Sup Vol) is less than half of the SMM volume (e.g., unconcentrated, original waste volume).
241-SX-109	2000	1966	Zero Solids. Adjusted 1966 SMM definition because of tank self-concentration effect. Used RSLT (R2) in SX tanks where the supernatant volume (Sup Vol) is less than half of the SMM volume (e.g., unconcentrated, original waste volume).
241-SX-110	1000	1976	Zero Solids. Unadjusted SMM definition for tank leak date of 1976.
241-SX-111[2]	500	1958	Zero Solids. Unadjusted SMM definition for tank leak date of 1958.
241-SX-112	1000	1969	Zero Solids. Adjusted 1969 SMM definition because of tank self-concentration effect. Used RSLT (R2) in SX tanks where the supernatant volume (Sup Vol) is less than half of the SMM volume (e.g., unconcentrated, original waste volume).
241-SX-113	15000	1958	Zero Solids. Unadjusted SMM definition for tank leak date of 1958.
241-SX-115	50000	1965	Zero Solids. Unadjusted SMM definition for tank leak date of 1965.
241-T-101	10000	1969	Zero Solids. Unadjusted SMM definition for tank leak date of 1969.
241-T-103	3000	1973	Zero Solids. Unadjusted SMM definition for tank leak date of 1973.
241-T-106	115000	1973	Zero Solids. Unadjusted SMM definition for tank leak date of 1973.
241-T-108[2]	1000	1957	Zero Solids. Unadjusted SMM definition for tank leak date of 1957.
241-T-109	1000	1974	Zero Solids. Unadjusted SMM definition for tank leak date of 1974.
241-T-111	1000	1971	Zero Solids. Unadjusted SMM definition for tank leak date of 1971.
241-TX-107	8000	1977	Zero Solids. Unadjusted SMM definition for tank leak date of 1977.
241-TY-101	1000	1973	Zero Solids. Unadjusted SMM definition for tank leak date of 1973.
241-TY-103	3000	1971	Zero Solids. Unadjusted SMM definition for tank leak date of 1971.
241-TY-104[2]	1400	1953	Zero Solids. Unadjusted SMM definition for tank leak date of 1953.
241-TY-105	35000	1957	Zero Solids. Unadjusted SMM definition for tank leak date of 1957.
241-TY-106	20000	1959	Zero Solids. Unadjusted SMM definition for tank leak date of 1959.
241-U-101	5000	1959	Zero Solids. Unadjusted SMM definition for tank leak date of 1959.

Table 3-2. Tank Farm Leak Event Sites and Definitions. (3 Sheets)

Tank	Volume (gal)	Year	Site Description
241-U-104	55000	1956	Zero Solids. Unadjusted SMM definition for tank leak date of 1956.
241-U-110	6500	1975	Zero Solids. Unadjusted SMM definition for tank leak date of 1975.
241-U-112	8500	1967	Zero Solids. Unadjusted SMM definition for tank leak date of 1967.

Notes:

[1]-According to Field and Jones (2005), losses in BY Tank Farm were not attributable to any specific tank. Appendix A discusses how these values were derived.

[2]-The leak declaration date in Hanlon (2004) is inconsistent with the tank traffic and volume data in Agnew et al. (1997b). Appendix A discusses the attribution of leak dates for these tanks.

As an example of the source tank leak description, the SMM output from the HDW Model for tank 241-C-111 in early 1968 is presented in Table 3-3. It had a 5500-gallon leak event defined, and this is the resulting SMM tank waste description from the HDW Model.

Table 3-3. Supernatant Mixing Model Tank Description Output. (3 Sheets)

Leak Year--1968	Site--241-C-111	Tank Traffic Volume
HDW Waste Stream	**Corresponding SIM Waste Stream**	**kgal**
MW1	MW1 (BT1)	0.00E+00
MW2	MW2 (BT2)	0.00E+00
1C1	1C1 (BT1)	2.13E-04
1C2	1C2 (BT2)	0.00E+00
2C1	2C1 (BT1)	0.00E+00
2C2	2C2 (BT2)	0.00E+00
224-1	224 (BT1)	0.00E+00
UR/TBP	TBP-UR (BT2)	1.56E-02
PFeCN1	PFeCN1 (BT1)	0.00E+00
PFeCN2	PFeCN2 (BT2)	0.00E+00
TFeCN	TFeCN (BT2)	3.99E+01
1CFeCN	1CFeCN (BT2)	0.00E+00
R1	R1 (R1)	0.00E+00
R2	R2 (R2)	0.00E+00
CWR1	CWR1 (CWR1)	0.00E+00
CWR2	CWR2 (CWR2)	0.00E+00
P1	PUREX P1 (P1)	0.00E+00
P2	PUREX P2 (P2)	0.00E+00
P2'	PUREX P2' (P2')	0.00E+00
PL1	PUREX PL1 (P1)	0.00E+00
CWP1	CWP1 (CWP1)	2.50E+02
CWP2	CWP2 (CWP2)	0.00E+00
CWZr1	CWZr1 (CWZr1)	0.00E+00
OWW1	PUREX (P1) Org Wst	8.03E-02

Table 3-3. Supernatant Mixing Model Tank Description Output. (3 Sheets)

Leak Year--1968	Site--241-C-111	Tank Traffic Volume
HDW Waste Stream	**Corresponding SIM Waste Stream**	**kgal**
OWW2	PUREX (P2) Org Wst	0.00E+00
OWW3	PUREX (P2') Org Wst	0.00E+00
Z	Z(Z2)	0.00E+00
HS	Sr-Cs Rec Wst (P1)_HS	2.28E+02
TH1	TH1 (TH2)	0.00E+00
TH2	TH2 (TH2)	0.00E+00
AR	Sr-Cs Rec Org Wst aqu(P2')_AR	0.00E+00
B	Sr-Cs Rec Org Wst (P2)_B	0.00E+00
BL	Sr-Cs Rec Org Wst aqu (P2)_BL	0.00E+00
SRR	Sr-Cs Rec Wst (P2)_SRR	0.00E+00
CSR in	N/A--source stream for CSR	0.00E+00
CSR	Sr-Cs Rec Org Wst (P2')_CSR	0.00E+00
DE	DE(NA)	0.00E+00
CEM	CEM(NA)	0.00E+00
NIT	NIT(NA)	0.00E+00
Salt Slurry	Salt Slurry(P2')	0.00E+00
DW	Decon Wst (P2)	0.00E+00
N	N Decon Wst (P2)	0.00E+00
BT in	N/A--source streams for BT-SltCk	0.00E+00
BT-SltCk	1C Evap (BT2)	0.00E+00
OrgSltCk in	N/A--source streams for OrgSltCk	0.00E+00
OrgSltCk	OrgSltCk(P2')	0.00E+00
R in	N/A--source streams for RSLT	0.00E+00
RSltCk	RSLT (R2)	0.00E+00
T2 in	N/A--source stream for T2SltCk	0.00E+00
T2-SltCk	T2-SltCk(P2')	0.00E+00
BY in	N/A--source stream for BYSLT	0.00E+00
BY-SltCk	BYSLT (BT2)	0.00E+00
S1 in	N/A--source streams for S1-SltCk	0.00E+00
S1-SltCk	S1-SltCk(P2')	0.00E+00
S2 in	N/A--source streams for S2-SltSlr	0.00E+00
S2-SltSlr	S2-SltSlr(P2')	0.00E+00
A1 in	N/A--source streams for A1-SltCk	0.00E+00
A1-SltCk	A1-SltCk(Z2)	0.00E+00
A2 in	N/A--source streams for A2-SltSlr	0.00E+00
A2-SltSlr	A2-SltSlr(Z2)	0.00E+00
P3AZ1	P3AZ1(P3)	0.00E+00
PL2	PUREX PL2 (P3)	0.00E+00
CWZr2	CWZr2 (CWZr2)	0.00E+00
P3AZ2	P3AZ2(P3)	0.00E+00
224-2	224 (BT2)	0.00E+00
PASF	PASF (P3)	0.00E+00

Table 3-3. Supernatant Mixing Model Tank Description Output. (3 Sheets)

Leak Year--1968	Site--241-C-111	Tank Traffic Volume
HDW Waste Stream	**Corresponding SIM Waste Stream**	**kgal**
WTR	PUREX (P2) Cool Wtr-Stm Cond; incremental dilution water was often removed (as in this case) for purposes of calculating contributing waste percentages	5.93E+00
GAS	N/A--estimated tank volume occupied by retained gas	0.00E+00
SWLIQ	N/A--saltwell liquor removed from tank	0.00E+00
UNK	N/A—unknown/unassigned waste volumes usually assigned as process water	3.71E+01
smmVol	Tank waste volume in original waste volume amounts	5.61E+02
supVol	Occupied tank liquid volume (includes concentration effects) at the time observed	4.45E+02
tlmVol	Occupied tank solid volume at the time observed	5.68E+01
tankVol	Effective occupied tank volume (supVol + tlmVol) at the time observed	5.02E+02

An example of how the SMM description is translated into SIM to be used in calculating an inventory is presented in Table 3-4. The volumes are translated into a percentage and then multiplied by the leak volume and parameterized.

Table 3-4. Example Tank Leak Event Description and Parameterization

Year	Tank	SIM Waste Stream	Total Volume Distribution (0 = Normal)	Mean Volume (ML)	Standard Deviation	Truncation level (0 = None)	Volume Percent Solids Distribution
1968	241-C-111	1C1 (BT1)	0	8.01E-09	1.00E-15	0	None
1968	241-C-111	TBP-UR (BT2)	0	5.86E-07	1.00E-15	0	None
1968	241-C-111	TFeCN (BT2)	0	1.50E-03	1.00E-15	0	None
1968	241-C-111	CWP1 (CWP1)	0	9.37E-03	1.00E-15	0	None
1968	241-C-111	PUREX (P2) Org Wst aqu_OWW1	0	3.01E-06	1.00E-15	0	None
1968	241-C-111	Sr-Cs Rec Wst (P1)_HS	0	8.56E-03	1.00E-15	0	None
1968	241-C-111	PUREX (P2) Cool Wtr-Stm Cond	0	1.39E-03	1.00E-15	0	None

(Note the small uncertainty assigned to achieve the practical result of minimizing the volume uncertainty contribution as described in Section 3.4.3)

3.3.3 Volume

Total volumes for disposal sites are usually closely measured, and the amount of uncertainty/variability associated with the total volume measurement is generally considered small. Waste volumes disposed to a particular location are assigned using available process knowledge/documentation where available. Uncertainties regarding waste volumes are usually quantified using a symmetrical triangular distribution. When information is contradictory or lacking regarding a site, waste volumes are assigned using general assumptions about the waste management practices of the time and boundary conditions of the production system during the waste location's operating life.

In these cases, where the overall volume is presented, but no specific breakout is found, surveillance and operations data are used and interpreted to develop waste stream definitions and the proportional waste volume assignments for the various sites. Where there is significant interpretation of the disposal records necessary to assign waste streams and volumes, higher uncertainties are assigned to those waste stream volumes contributing to those sites.

The principal source for identifying disposal sites and UPRs, their disposal volume, waste stream assignment, and site location information is the Waste Information Data System (WIDS) database (DOE-RL 2002). Where a volume and waste stream are provided in the reference, those parameters are used. For the more uncertain situations, a waste stream is deduced from the WIDS narrative, relying on the proximity to a particular facility or waste tank (in most cases, a waste stream or waste source is called out and matched to the available waste streams in SIM) and timing of the loss. In the case of unplanned releases, Appendix A, Section A5.3 presents the loss volume quality level bin (1 – 4) which is assigned commensurate with the level of information provided in WIDS (DOE-RL 2002) when defining the mean volumes and volume uncertainties associated with the more ambiguously described unplanned releases. These categories describe the available information and determined how waste types, quantities, and uncertainties are established. The quantities estimated in these cases are considered initial values requiring additional evaluation/analysis.

Liquid waste disposal sites and unplanned releases generally have waste type and volume assignments available from historical information. The case of the tank and ancillary equipment leaks represents a special case of using the HDW Model and applying process engineering knowledge from Field and Jones (2005) and elsewhere. The volumes of the tank farm leaks were specified in the reference, but because the liquids in the tanks are blended, leak-specific compositions and component volumes are not readily available. Therefore, a certain amount of technical judgment and additional information are used to define the composition of the tank leak. Deducing this other information was especially important for modeling the tank conditions if environmental factors, such as self-concentration, needed to be accommodated as part of the leak description, or if the leak date was ambiguous. As described in Section 3.3.2, the supernatant mixing model (SMM) subroutine of the HDW Model is run up to a specific point in history allowing a highly specific tank composition to be derived for that tank at that point in time with the waste streams apportioned to the established leak volume by percentage. Thus, using the waste stream definitions, the leak date, tank process history, and the established volume as a basis, an inventory for the leak was developed.

Very few waste streams disposed to the past-practice sites are considered to possess solids because of the waste management and surveillance practices employed during production operations and the general physical constraints of the system with regard to particulate entrainment (radiation monitors, settling tanks, no agitation, passive filtration, etc.). Thus, the default condition for SIM Rev. 1 is not to incorporate entrained solids. However, for certain waste streams and waste sites, the inclusion of entrained solids is reasonable from a physical and waste management operations perspective—laboratory waste, decontamination waste, various process cold start waste, and fuel fabrication waste are all likely to have solids. In addition, selected process excursions where the conventional waste management practices are deemed inadequate to maintain containment are also considered as part of this evaluation (piping failures, overflow conditions, or poor in-tank settling).

In those few cases where solids are included, significant data analysis and/or data manipulation is sometimes necessary to parameterize the volume percent solids quantity. Some analytes (e.g., uranium, strontium-90, plutonium) existed in waste streams almost entirely in the solid phase and were present in waste streams in high concentrations (in the absence of organic complexants) only if entrained. Thus, the site inventory of one or more of these analytes is often used to determine the volume percent solids content of a contributing waste stream, while endeavoring to maintain the analyte inventory correlation inherent in the waste site reference data.

3.4 UNCERTAINTY PARAMETERIZATION

As part of the waste stream definition task, refinements for the uncertainty assumptions for analytes without measurement were developed, as well as further evaluation and description of those waste stream inputs with some data. The SIM parameters used in developing inventory, (density, volume, volume percent solids, and concentration) are strictly non-negative; therefore, the distributions used to represent the physical and chemical features of the waste must correspond to this physical constraint.

A larger suite of uncertainty descriptions is available to describe the waste stream compositions in this version of SIM than in the prior version, and significantly larger uncertainties are associated with the individual component volumes at some of the disposal sites. Uncertainties for each input component in the inventory calculation (concentration, density [liquid and solid in both cases], total volume, and volume percent solids) are assumed or derived. For each component, there are nine different distribution types available from which to select to describe an assumption. Each distribution has up to three parameters defining the limits of the uncertainty distribution. The new assumptions replaced the arbitrary placeholder values that were used initially (Simpson et al. 2001). The assumptions currently used are now generally traceable back to physical and chemical principles or documented operating guidelines in the absence of appropriate data.

The number of available distributions from OCB was limited after review and evaluation of the various source data. Although specific data-based distributions could have been derived in certain cases, the necessary modifications to the model architecture and properly accommodating

the inconsistencies that exist between the varieties of data sets to be incorporated would have diminished the technical defensibility of the model and increased the complexity of the uncertainty derivation and assignment process without enhancing the technical quality of the output. Additionally, the curve fit agreement statistics in many cases are not very high regardless of the distribution types evaluated. Therefore, the SIM uncertainties were restricted to this basis set, using the analysis of the available data to guide the selection.

Distributions for modeling parameters and their quantitative descriptions are assigned by a variety of methods. The distributions are then interpreted by the OCB.Net Library by the "distribution type" index and the associated parameters (also referred to as Parms) as seen in Table 3-5 (parameter 1, parameter 2, and parameter 3, which are different depending on the distribution). All input cells must be filled with the appropriate values (parameters 1 through 3) to define a distribution, or if a distribution does not use three parameters, zero (0) must be entered in the remaining cells to allow the simulation calculations to proceed.

Table 3-5. Available Distribution Parameter Definitions

Distribution Type Index	Distribution Name	Parameter 1	Parameter 2	Parameter 3
0	Normal	mean	standard deviation	low cut-off
1	Triangular	minimum	mode	maximum
4	Lognormal	mean	standard deviation	high cut-off
6	Exponential	rate	0 = none	0 = none
8	Weibull	location	scale	shape
9	Beta	alpha	beta	scale
12	Gamma	location	scale	shape
17	Zero (null)	0	0 = none	0 = none
18	1 (unity)	1	0 = none	0 = none

For a greater understanding of each type of distribution and their definition in OCB, refer to Decisioneering's website at http://www.decisioneering.com. For the purposes of describing uncertainty magnitude in the context of output in this model, relative standard deviation (RSD), which is the standard deviation of the distribution divided by the mean, is considered to be the metric, unless otherwise specified.

3.4.1 Density Uncertainty Assignment

The assumed uncertainty parameter definition is a function of mean density in both phases. The derived definition from these boundary conditions is a lognormal distribution ranging from 1% to 5% RSD of the mean. This assignment depends on where the density for a particular waste stream falls within the range of observed values (e.g., waste streams with simple compositions that are mostly water have the smallest uncertainties, with the density uncertainty increasing as a function of the waste stream composition complexity).

The solids are considered to be simple, single-phase homogeneous mixtures of material. No speciation was assumed; thus, a lognormal distribution with a 5% RSD around the mean was conventionally assumed for all solids densities. These ranges follow the generally observed limits of bulk density behavior for these liquids and solids.

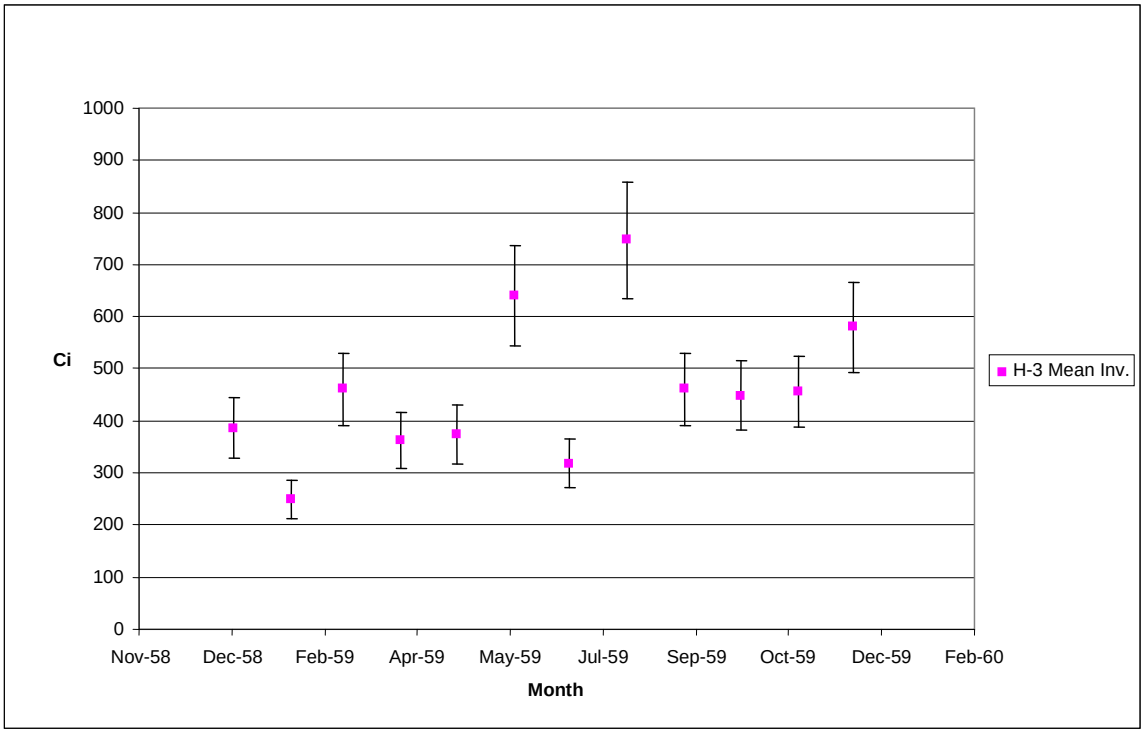
3.4.2 Waste Stream Composition (Concentration) Uncertainty Assignment

In measurements of Hanford Site waste streams, the distributions of the data are often found to be skewed and have long tails. These chemical data are usually best represented by lognormal distributions. In other cases, a different distribution selection is indicated. The triangular distribution is used when there is a paucity of data points for waste stream composition but there is a typical range of values suggested by the historical data. Zero is used where process knowledge indicates that the analyte is not present. Appendix A presents further discussion regarding the derivation and treatment of concentration uncertainty.

Waste stream uncertainties associated with chemical inputs are considered relatively simple and modest—the distribution types thought to best represent these components are lognormal, triangular, or zero, with RSDs generally ranging in magnitude from 7% to 64%. In most cases, the HDW Model estimated production variabilities are used to define uncertainties. These uncertainties are mostly associated with process definition, performance, or measurement and these distributions are thought to appropriately describe underlying physical or chemical conditions being modeled. Some of the larger waste stream uncertainties are associated with more complicated interactions involving reprocessed or reworked wastes with the introduction of organic complexants, such as uranium recovery wastes or various B Plant fission product reprocessing wastes (Agnew et al. 1997a).

Because of the incomplete nature of the uncertainty data available from current characterization or historical process chemistry data, a consistent, comprehensive, and reproducible set of uncertainties is required to perform the modeling calculations. Uncertainties for most of the individual radionuclide estimates for a particular fuel element obtained from ORIGEN2 are relatively small (Wootan 1998; Heeb 1991) and at the annual level, the variability does not appear to be excessive. Figure 3-1 illustrates an example of the annual production variability for tritium in 1959 using the ORIGEN 2 data, incorporating error bars to demonstrate the conventional assumption regarding uncertainty at the individual (i.e., monthly production) level.

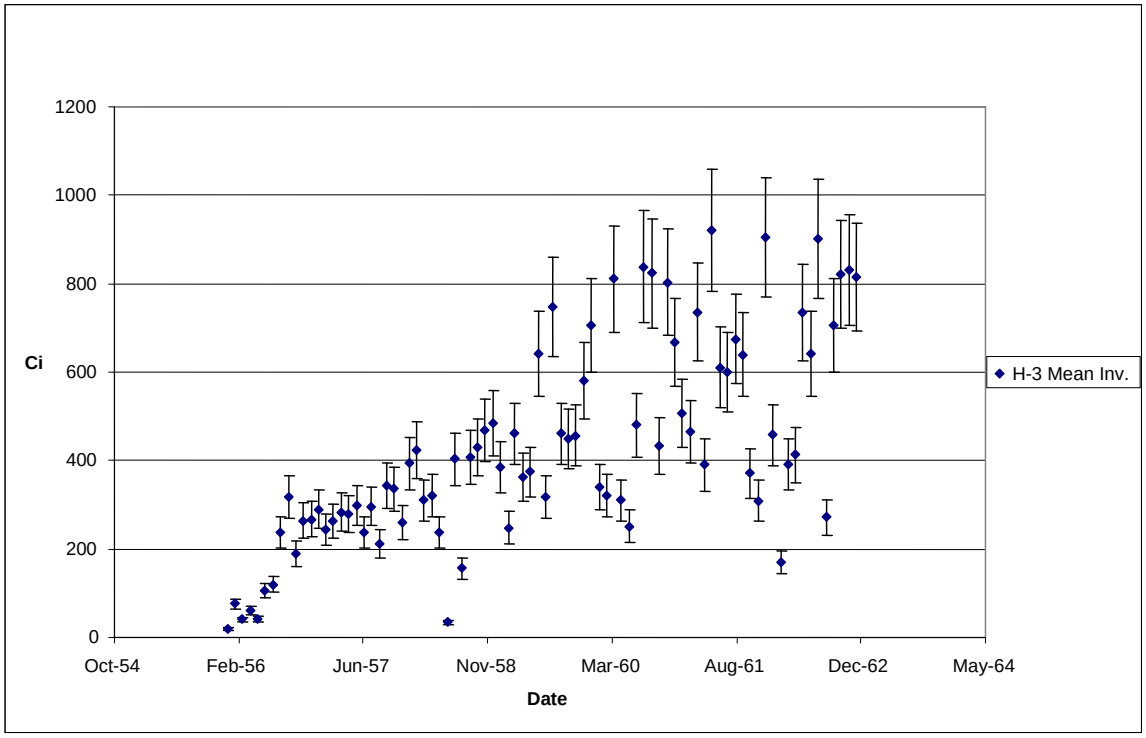
Figure 3-1. Tritium Inventory through PUREX in 1959[1]



([1]Watrous et al. 2002)

However, the analyte uncertainties are not quantified at that level of resolution. Instead, the guiding assumption is that the reactor production variability as a function of time would be a reasonable proxy for describing uncertainty. The production variability data is pooled by separation process in five to seven year increments, mirroring the division in the HDW Model, and providing a sufficient number of observations in each increment to run the Crystal Ball distribution fitting program. This segregation scheme is also used to keep from cross-contaminating the separate inventory source terms to maintain the global mass balance and to keep the appropriate pooled variability assumptions together with the appropriate waste streams. Figure 3-2 illustrates the uncertainty/variability in an example involving tritium in the overall early PUREX production regime (P1).

Figure 3-2. Tritium Inventory through PUREX (1956-1962)[1]



([1]Watrous et al. 2002)

It is not clear from the available data whether the solubility behavior should be considered separately for deriving uncertainty or if the uncertainty described by the ORIGEN2 curve fit data satisfactorily encompasses the range of possible values. In this case, the Crystal Ball data-fitting treatment of the derived beta distributions could be considered the most conservative quantification interpretation for this distribution because the lower limit in this treatment always includes zero, resulting in broader uncertainties. Additionally, this method of calculating uncertainties may represent the uncertainty as being larger on an annual basis than it actually is because the calculated data set is more variable as a whole than for any particular year.

For now, the ORIGEN2 production data are considered to envelop any uncertainty introduced by chemical behavior. Thus, to derive the radionuclide uncertainties for use in SIM, for both measured and unmeasured analytes, the outputs from ORIGEN2-DKPRO (Watrous et al. 2002) were divided into campaigns as a function of time and separation plant corresponding to the overall Hanford Site operating history.

Statistical distributions and quantitative descriptions for each radionuclide inventory for each campaign were then fitted to these results. A key assumption was then made: ***The radionuclide uncertainties associated with the campaign inventories are considered to describe the individual waste stream uncertainties; thus, the assumption was made that waste stream uncertainty descriptions can be scaled from the resulting inventory uncertainty distributions via transformations of the distribution around the desired mean waste stream analyte***

concentration. Furthermore, the uncertainty behavior for the individual analytes would be indifferent to phase (e.g., similar analyte uncertainty behavior is attributed to both solids and liquids). Table 3-6 describes the various categories of uncertainty designation and what data was fit to provide the beta distribution definitions.

Table 3-6: Uncertainty Distribution Categories

Uncertainty Designation	Source Data Definition
BT1	ORIGEN2 data associated with the fuel rod dissolution in the early bismuth phosphate process (1944-1949)
BT2	ORIGEN2 data associated with the fuel rod dissolution in the later bismuth phosphate process (1950-1956)
R1	ORIGEN2 data associated with the fuel rod dissolution in the early REDOX process (1952-1958)
R2	ORIGEN2 data associated with the fuel rod dissolution in the early REDOX process (1959-1966)
P1	ORIGEN2 data associated with the fuel rod dissolution in the early PUREX process (1956-1962)
P2	ORIGEN2 data associated with the fuel rod dissolution in the PUREX process (1963-1967)
P2Prime	ORIGEN2 data associated with the fuel rod dissolution in the PUREX process (1968-1972)
P3	ORIGEN2 data associated with the fuel rod dissolution in the PUREX process (1983-1990)
Z1	Composite of ORIGEN2 data from BT2, R1, and P1
TH2	Composite of ORIGEN2 data associated with the fuel rod dissolution in the Thoria process wastes (1966 and 1970)
CWBT1	ORIGEN2 data associated with the cladding dissolution in the early bismuth phosphate process (1944-1949)
CWBT2	ORIGEN2 data associated with the cladding dissolution in the later bismuth phosphate process (1950-1956)
CWR1	ORIGEN2 data associated with the cladding dissolution in the early REDOX process (1952-1958)
CWR2	ORIGEN2 data associated with the cladding dissolution in the early REDOX process (1959-1966)
CWP1	ORIGEN2 data associated with the Al-cladding dissolution in the early PUREX process (1956-1962)
CWP2	ORIGEN2 data associated with the Al-cladding dissolution in the PUREX process (1963-1967)
CWZr1	ORIGEN2 data associated with the Zr-cladding dissolution in REDOX and PUREX (1968-1972)
Z2	Composite of ORIGEN2 data from R2, P2, and P2Prime
CWTH2	Composite of ORIGEN2 data associated with the cladding dissolution in the Thoria process wastes (1966 and 1970)
CWZr2	ORIGEN2 data associated with the Zr-cladding dissolution in PUREX (1983-1989)
NA	Uncertainty assignment to non-radioactive waste streams (not applicable)

3.4.3 Volume Uncertainty Assignment

Liquid waste disposal sites often had documented the volume of individual waste streams disposed during each year of operation. General rules for volumetric uncertainty assignment used for application in SIM are:

1. A symmetric triangular distribution with an uncertainty of 10% is assigned where documentable site and volume information available;
2. A symmetric triangular distribution with an uncertainty of 25% is assigned where a total volume was available for the site operating history but where volume measurements as a function of time are intermittent and have to be estimated or volumes apportioned between contributing waste streams;
3. A symmetric triangular distribution using a linearized volume estimate with an uncertainty of 50% is assigned where a total volume is available for the site over a number of years but no individual volumes as a function of time are available.

Unplanned release sites are the result of a variety of infrastructure failures that occurred during the production mission at the Hanford Site. For developing unplanned release volumes, a series of bins (Quality Levels 1-4) was established to segregate the amount and quality of information regarding various events. The bins then establish the uncertainty parameters applied to the volume or in many cases, establish a method to quantify a mean volume and then parameterize an uncertainty for that value.

Where documented volumes are available from the surveillance data sources cited in Section 8.0, they are used and a modest uncertainty (similar to the uncertainty applied to a disposal site) is applied. For the more uncertain situations that were incorporated into SIM Rev. 1, a waste stream is deduced from the WIDS (DOE-RL 2002) narrative, relying on the proximity and timing to a particular facility or waste tank (in most cases a waste stream or waste source is called out and matched to the available waste streams in SIM) and a distribution applied. Appendix A, Section A5.3, presents the specifics regarding the assignment and derivation of the mean volumes and uncertainties for the unplanned releases.

- In Quality Level 1, a specific volume and type of waste is called out in the record. This situation is assigned a triangular distribution with 10% variability, similar to a well defined disposal site.
- In Quality Level 2, a waste stream is indicated together with a set of geographic dimensions that define the unplanned release area. A modified beta distribution that resembles a uniform distribution ranging from zero to twice the mean volume is assigned to account for the various uncertainties that are incorporated into this estimate.
- In Quality Level 3, a total Ci or mass (in g/kg) amount of an analyte/radionuclide is provided. Because of the general descriptions provided regarding the activity, a mean volume is calculated from a likely waste stream and a lognormal distribution with 100% relative standard deviation is assigned.

- In Quality Level 4, there is no specific quantitative information, but there are other qualitative descriptions regarding the loss (such as a visual report of waste pooling). In these cases where qualitative information indicated that a loss of waste occurred, but no reliable volume estimate made, a rough order of magnitude value was developed for the mean volume and an exponential distribution was assigned.

Development of the uncertainties associated with the volumes connected to the tank farm leaks was substantially different from the methods used to evaluate and assign disposal site uncertainties. Field and Jones (2005) established volumes associated with each leak event. Sensitivity analysis and uncertainty associated with tank farm leak volumes will be addressed in the upcoming Single-Shell Tank (SST) Performance Assessment (PA). Thus, at the direction of Tank Farms personnel (Jones 2005), minimal volume uncertainties were incorporated into the SIM Rev. 1 modeling effort. Therefore, the volumes for these events are described using normal distributions around the reference values (Field and Jones 2005) with extremely small standard deviations when performing the inventory calculation in SIM Rev. 1. Decisions regarding the volumetric uncertainties associated with the SST PA activity will be established and incorporated into SIM at a later time.

Because few waste streams disposed to the past-practice sites are considered to possess solids and the conditions that foster solids formation and entrainment are highly variable and not well-understood, the uncertainty for most waste streams with volume percent solids is represented as an asymmetric triangular distributions with a minimum and a mode set to zero and an upper limit that is considered bounding from physical and site inventory constraints. In select situations, there is sufficient context to assign a different distribution (such as symmetric triangular, normal, or lognormal) for a waste stream-disposal site combination; however, these cases prove to be the exception.

3.5 CORRECTION FACTORS (CORRFACTORS SPREADSHEET)

The *CorrFactors* contains scalar values that are used to convert units of the analyte inventories calculated in SIM to those desired by SAC. The units selected for the input data to perform the calculation provide results in kg on a mass basis and kCi on an activity basis. However, because of a characteristic in the OCB® code, the very small concentration values (values less than 1E-16 μCi/g) for some of the radionuclide values do not compute when defining distributions for SIM during initialization. Thus, the input concentration values for the radionuclides are inflated by 1E+09 so that the distribution definition step can proceed and the remainder of SIM execute. When reporting the results, all radionuclide results are multiplied by 1E-06 to correct for this initialization step and provide output results in curies. Because of the units selected for the chemical inventory calculation and because there are no chemical concentrations less than 1E-16, no inflation factor is applied and the correction factor for those analytes is 1 to provide output in kilograms.

4.0 MODEL ARCHITECTURE

SIM Rev. 1 was developed to perform a Monte Carlo simulation with 25,000 trials per input parameter for each selected soil waste site using the liquid and solid waste stream composition definitions and waste site descriptions. There are two discrete pieces of SIM that work together to generate inventory and uncertainty estimates: (1) the SIM production workbook file (*SIMInput_Base*), which is the source data file and the principal output summary reporting file; and (2) the executable file (**OCBHanford**), which administers the execution of the model, performs the calculations, and manages the data reporting. Other elements of SIM involve the input definition process discussed in Section 3.0, input parameters discussed in Section 4.1.1, and post-process data analysis discussed in Section 5.0.

The selected modeling architecture enhances the speed, versatility, and reliability of SIM over other architecture options. The speed of simulation over other previous methods to compute inventories with uncertainties at the Hanford Site is substantial because of recent improvements in hardware and software, although a fully converged SIM output requires several days to complete. The highly robust, modular structure of this model allows the inputs and assumptions to be modified quickly and easily, allows the model to be scaled up to add more waste streams and waste sites as needed (within certain hardware and software constraints), or allows it to be adapted to new scenarios. Furthermore, the familiar Excel interface for output analysis and the ability to run this model on conventionally available personal computers are significant advantages.

4.1 MODEL METHOD

This section will briefly address the theory underlying the Monte Carlo method of stochastic simulation used in SIM. Monte Carlo is the method of approximating an expectation by the sample mean of a function of simulated random variables. It is about invoking laws of large numbers to approximate expectations, where the simulated random variables are independent. In mathematical terms, consider a random variable X having probability mass function or probability function $f_X(x)$ which is greater than zero on a set of values χ. Then, the expected value of a function g of X is:

$$\mathbb{E}(g(X)) = \sum_{x \in \mathcal{X}} g(x) f_X(x) \qquad \text{(Equation 4.1)}$$

if X is discrete and

$$\mathbb{E}(g(X)) = \int_{x \in \mathcal{X}} g(x) f_X(x) dx \qquad \text{(Equation 4.2)}$$

if X is continuous. Now, if an *n*-sample of X's, (a, b, c, …), and the mean of g(x) is computed over the sample, then that would result in the Monte Carlo estimate

$$\tilde{g}_n(x) = \frac{1}{n}\sum_{i=1}^{n} g(x_i) \quad \text{of } \mathbb{E}(g(X)). \qquad \text{(Equation 4.3)}$$

Alternately, the random variable,

$$\tilde{g}_n(X) = \frac{1}{n}\sum_{i=1}^{n} g(X) \qquad \text{(Equation 4.4)}$$

can be considered the Monte Carlo estimator of $\mathbb{E}(g(X))$.

If $\mathbb{E}(g(X))$ exists, then the weak law of large numbers indicates that for any arbitrarily small ϵ

$$\lim_{n\to\infty} P\left(|\tilde{g}_n(X) - \mathbb{E}(g(X))| \geq \epsilon\right) = 0. \qquad \text{(Equation 4.5)}$$

This equation indicates that as *n* gets large, then there is a small probability that $\tilde{g}_n(X)$ deviates much from $\mathbb{E}(g(X))$. For the purposes of this task, the strong law of large numbers says that so long as *n* is large enough, $\tilde{g}_n(X)$ arising from the Monte Carlo calculation shall be as close to $\mathbb{E}(g(X))$ as desired. In this case, 25,000 trials were determined to be a sufficiently large number to provide a satisfactory estimate of both the mean and the behavior of the output distribution throughout its range. For further detail regarding Monte Carlo methods, a principal reference cited in the Crystal Ball documentation is Hammersley and Handscomb (1964).

4.1.1 Model Inputs

All input data were entered into the various Excel worksheets. The .Net C# (dot-Net C-Sharp) interface code extracted the necessary information from the input spreadsheets to perform calculations as needed. There were four spreadsheets used to collect and organize input data in the SIM production workbook (i.e., *SimInput_Base*) file. They are named *SiteInput, AnalyteInput, DensityInput,* and *CorrFactors.* Each is discussed in the following paragraphs. These spreadsheets contain the assumptions required for the calculation (e.g., the quantitative information describing the input values and their corresponding distributions used in the model).

For the purpose of clarity, an assumption in OCB is an input value for a modeling parameter (density, volume, concentration) together with its uncertainty definition (e.g., the type of distribution and its quantitative description), as opposed to the technical suppositions and simplifications that underlie overall SIM development. There are additional output and data analysis worksheets that are part of the production workbook file. These will be discussed later in Section 5.0.

SIM is based on the following input data, represented by matrices:

Model Input Matrix		**Workbook Location**
$\mathbf{CL}_{(i,k)}$:	concentration liquid matrix;	*AnalyteInput* worksheet
$\mathbf{CS}_{(i,k)}$:	concentration solid matrix;	*AnalyteInput* worksheet
$\mathbf{TV}_{(j,k,l)}$:	total volume matrix;	*SiteInput* worksheet
$\mathbf{VP}_{(j,k,l)}$:	volume percent solids matrix;	*SiteInput* worksheet
$\mathbf{CFL}_{(i)}$:	correction factor liquid matrix;	*CorrFactor* worksheet
$\mathbf{CFS}_{(i)}$:	correction factor solid matrix;	*CorrFactor* worksheet
$\mathbf{DL}_{(i,k)}$:	density liquid matrix;	*DensityInput* worksheet
$\mathbf{DS}_{(i,k)}$:	density solid matrix;	*DensityInput* worksheet

i = number of chemicals or radionuclides;	$i=1,i_{max}$	i_{max} = 75 analytes
j = number of sites;	$j=1,j_{max}$	j_{max} = 377 total sites
k = number of waste streams;	$k=1,k_{max}$	k_{max} = 196 waste streams
l = years of operation	$l = 1944, l_{max}$	l_{max} = 2001 calendar year

The inventory calculations follow the example below. Each parameter has an input distribution for each i, j, k, and l that serve as inputs to the simulation. In this simulation of 25,000 trials, a random selection from each independent input distribution is used to calculate inventory and the resulting matrices are computed. The collections of forecasted outputs are then exported into a series of Excel workbooks. Summary outputs for each site are exported back into the production workbook file; individual site outputs are organized by operable unit and results are reported in separate workbooks.

$\mathbf{FL}_{(j,i,l,)}$: forecast liquid matrix; $\mathbf{FL}_{(j,i)} = \mathbf{FL}_{(j,i)} + \mathbf{CL}_{(i,k)} * \mathbf{DL}_{(i,k)} * \mathbf{TV}_{(j,k,l)} * [1-\mathbf{VP}_{(j,k,l)}] * \mathbf{CFL}_{(i)}$

$\mathbf{FS}_{(j,i,l)}$: forecast solid matrix; $\mathbf{FS}_{(j,i)} = \mathbf{FS}_{(j,i)} + \mathbf{CS}_{(i,k)} * \mathbf{DS}_{(i,k)} * \mathbf{TV}_{(j,k,l)} * \mathbf{VP}_{(j,k,l)} * \mathbf{CFS}_{(i)}$

$\mathbf{FT}_{(j,i,l)}$: forecast total matrix; $\mathbf{FT}_{(j,i)} = \mathbf{FT}_{(j,i)} + \mathbf{CL}_{(i,k)} * \mathbf{DL}_{(i,k)} * \mathbf{TV}_{(j,k,l)} * [1-\mathbf{VP}_{(j,k,l)}] * \mathbf{CFL}_{(i)} + \mathbf{CS}_{(i,k)} * \mathbf{DS}_{(i,k)} * \mathbf{TV}_{(j,k,l)} * \mathbf{VP}_{(j,k,l)} * \mathbf{CFS}_{(i)}$

Deterministically:

$$F^{L}_{i,j,l} = Corr^{L}_{i} * (\Sigma_k \mathbf{C}^{L}_{i,k} * \mathbf{D}^{L}_{i,k} * \mathbf{TV}_{j,k,l} * [1-\mathbf{VP}_{j,k,l}])$$
$$F^{S}_{i,j,l} = Corr^{S}_{i} * (\Sigma_k \mathbf{C}^{S}_{i,k} * \mathbf{D}^{S}_{i,k} * \mathbf{TV}_{j,k,l} * \mathbf{VP}_{j,k,l})$$
$$F^{T}_{i,j,l} = F^{L}_{i,j,l} + F^{S}_{i,j,l}$$

Stochastically:

$$F^{L}_{i,j,l,t} = Corr^{L}_{i} * (\Sigma_k \mathbf{C}^{L}_{i,k,t} * \mathbf{D}^{L}_{i,k,t} * \mathbf{TV}_{j,k,l,t} * [1-\mathbf{VP}_{j,k,l,t}])$$
$$F^{S}_{i,j,l,t} = Corr^{S}_{i} * (\Sigma_k \mathbf{C}^{S}_{i,k,t} * \mathbf{D}^{S}_{i,k,t} * \mathbf{TV}_{j,k,l,t} * \mathbf{VP}_{j,k,l,t})$$
$$F^{T}_{i,j,l,t} = F^{L}_{i,j,l,t} + F^{S}_{i,j,l,t}$$

Where *t* = one trial

The currently reported output contains the mean, median, standard deviation, and twenty-one percentiles (0.5, 5, 10,…95 and 99.5) that can be used to define distributions for input to the SAC. These percentiles were chosen for their ability to comprehensively describe a distribution that encompasses 99% of the area within the resulting distribution, but the user can select different percentiles as desired or necessary. The output results are organized by closure zone and can be found in Appendix C (an electronic appendix to this document). The results presented are totals for the entire waste volume and the individual liquid and solid phase inventory contributions for each site. This functionality was included for potential transport modeling as well as for anticipated future SAC requirements.

The mean was the selected measure of central tendency; thus, the SIM outputs used for comparison are the means of the modeling results. However, the median is also routinely reported as well and may be more appropriate in other evaluations. Outputs are reported in kilograms or curies.

Volume input data were reviewed and modeling parameters developed. These definitions were converted into a standard electronic format, the *SiteInput* spreadsheet of the SIM workbook. The volume assumptions are particular to the site, year, and waste stream that contributed to the inventory. The complete data record used in the model includes the site label, year, waste stream label, total volume, and volume percent solids, which are entered in the subsequent columns of this spreadsheet, respectively. Input volumes are measured in megaliters (ML). The waste site and waste stream indices correspond to the identification number in the *Legend* spreadsheet. The volume definition (total volume and volume percent solids, waste stream assignments, and their respective distributions) has eight columns providing the quantitative information about the amount and uncertainty associated with a particular waste stream for each site-year combination. Each site has a unique combination of waste stream and year descriptions assigned. Table 4-1 provides an example of the structure of the volume input matrix. Each distribution type definition is previously described in Table 3-5 in Section 3.4.

Table 4-1. *SiteInput* Worksheet Example

Legend #	Legend #					Total Volume (ML)				Vol % Solids		
s	w	Site	Year	Waste Stream	Dist Type	Parm 1	Parm 2	Parm 3	Dist Type	Parm 1	Parm 2	Parm 3
1	45	200-E-100	1945	BiPO4 (BT1) Cool Wtr-Stm Cond	1	0.00219	0.00438	0.00657	17	0	0	0

After the sites for analysis in SIM were selected, the waste streams necessary to compute inventory (and associated uncertainty) were defined. Each waste stream has its own qualitative and quantitative description derived from historical process engineering data, assumptions regarding the presence and behavior of various analytes, and the previously developed waste stream values. The waste stream and analyte indices correspond to the identification number in the *Legend* spreadsheet. The *AnalyteInput* spreadsheet in the SIM workbook defines the

quantitative information about concentration and uncertainty behavior of a specific analyte (or radionuclide) within a waste stream. Table 4-2 presents an example of the structure of the *AnalyteInput* worksheet.

Table 4-2. *AnalyteInput* Worksheet Example

Legend #	Legend #				Derivation worksheet Liquids Input (µg/g or µCi/g; radionuclides *10e9)				Derivation worksheet Solids Input (µg/g or µCi/g; radionuclides *10e9)		
w	a	Waste Stream_ Unc	Analyte	Dist - liquid	Parm1	Parm2	Parm3	Dist - solid	Parm 1	Parm 2	Parm 3
1	1	1C Evap (BT2)	Na	4	8.99E+04	1.40E+04	3.43E+05	4	1.78E+05	2.77E+04	6.78E+05

As part of the data development process, separate working files were used to store, develop, manipulate, and consolidate composition and uncertainty data prior to its loading into the model. These development files were worksheets that were consolidated into a waste stream workbook (WSWB). These worksheets and their associated parameterization equations and links were used to structure and automate many aspects of data development and SIM interaction. All of the HDW waste streams used are contained in the WSWB file. Appendix D is an electronic appendix that is part of this document and contains the production inputs used in SIM, including the WSWB.

The WSWB file was developed over time and structured to contain a working copy and production copy of all the waste streams used. The working copy contained any necessary comments, references, or manipulations performed to compute the production waste stream compositions. The production copy is a consolidated output worksheet that incorporates the necessary parameterizations so that the comprehensive waste stream list is ready to be used in SIM.

The *DensityInput* spreadsheet of the SIM workbook defines the density of a specific waste stream. In this case, the guiding assumption is that all analytes have the same density within a waste stream phase (e.g., a separate bulk density is assumed for solids and liquids in a waste stream); thus, the density will be defined only by the specific waste stream and phase. Densities used in waste stream definitions were derived from cited sources. The waste stream index corresponds to the identification number in the *Legend* spreadsheet with the waste stream label. The mean values and distribution definitions for the supernatants and the solids are defined in the subsequent columns. Table 4-3 presents an example of the *DensityInput* worksheet.

Table 4-3. *DensityInput* Worksheet Example

Legend #		Supernatants	Density (g/mL)			Solids	Density (g/mL)		
w	Waste Streams—current	dist type	Parm 1	Parm 2	Parm 3	dist type	Parm 1	Parm 2	Parm 3
1	1C Evap (BT2)	4	1.26	0.063	0	4	1.77	0.088	0

Because many of the liquid waste streams were dilute, a mean density of 1.01 g/mL (with a lognormal distribution having a standard deviation of 0.01) was used to define many of them. Uncertainties for the waste stream phase densities were based on simple physical and chemical considerations and in general had a relatively narrow range.

4.1.2 Executable Files

SIM Rev. 1 uses several executable files in various stages to generate inputs and outputs. The principal executable file is the **OCBHanford** interface application**. OCBHanford** is the executable file containing the C# code that creates the probability distributions, performs the inventory calculations, manages the data reporting, and creates the output files. The **OCBHanford** dialog box also presents a series of diagnostic data regarding simulation time and computing resources demand that can be useful in gauging hardware suitability and model parameter settings.

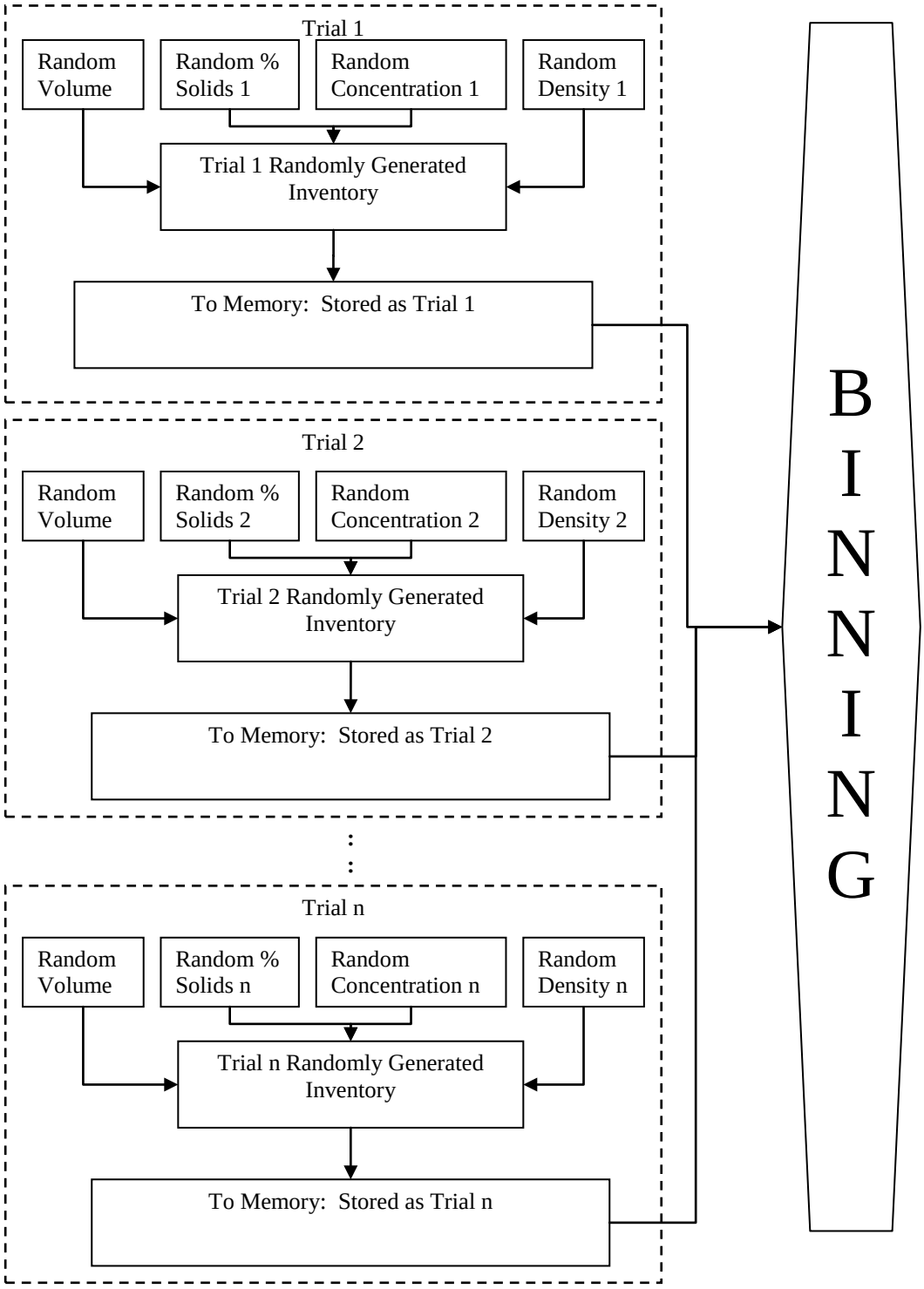
On activation of **OCBHanford**, a dialog box appears. This dialog box is the means to select which *SIMInput_Base* file will be used to perform inventory estimates. The dialog box has only one drop-down menu command, which is "File," and from there the file to be used must be selected. Once selected, there are a couple of actions that can be taken. The *SIMInput_Base* file can be checked for inconsistencies or errors by checking the appropriate box, and selecting "Test Distributions." The code will then review the various input definitions and assign the index identification numbers used by the interface to organize and calculate the results. If there is an error or problem with the *SIMInput_Base* file, a series of message boxes will appear describing them and their location within the workbook.

During initialization of the model, several actions occur. The site labels in the *SiteInput* spreadsheet are matched to the site labels in the *Legend* spreadsheet and indexed to their specific site identification numbers from the *Legend* spreadsheet. These indices are assigned to the first column of the *SiteInput* sheet and are used by the OCB user interface in executing and administering the calculation. Similarly, the waste stream labels in the *SiteInput* spreadsheet are matched to the waste streams in the *Legend* spreadsheet and indexed to their specific waste stream identification number from the *Legend* spreadsheet and assigned the waste stream identification numbers to the second column of the *SiteInput* sheet.

Once the model is initialized, if the file is satisfactory, unchecking the box and selecting "Calculate" will activate SIM and calculation will commence. If during a simulation a problem is discovered or if the user has a need, there are "Pause" and "Cancel" commands that will alternately temporarily suspend the simulation or stop and quit the application entirely as desired. As the simulation progresses and inventory results are generated, **OCBHanford** creates numerous temporary "bins" in resident memory as a function of the number of percentiles being reported into which results for each site-year-analyte combination are allocated. Figure 4-1 illustrates the inventory computation and binning process. The output statistics for inventory are based on the results in these bins for a site as a function of time and for the level of resolution being reported. Each analyte-year combination is independently calculated and reported for a site; however, the analyte results for a site over time are also accumulated. The summary analyte results developed for the site over its operating life result in a distribution for all the contributing

years. In this case, each term in the inventory calculation has 25,000 random outcomes generated within the defining distribution which are then used in computing inventory.

Figure 4-1. Illustration of Inventory Generation and Binning Process



As part of the calculation of the output inventories, the ordered outcomes are maintained in these bins. This data management process is repeated and maintained at each level of resolution (each site over a number of years, for each site as a function of its operable unit membership, and for the overall system) for each analyte; hence SIM's need for significant memory and computing power. The resulting summary statistics and percentiles are obtained from the "binned" outcomes, as a function of time, location, and model resolution. Table 4-4 illustrates an example of this organization and data management process.

Thus, one cannot simply sum the percentile outcomes for a site over time (or the percentiles for a series of sites in a closure zone) and generate the resulting output distribution correctly, although summing the means over a series of years will provide the correct overall site mean. Each site-year-analyte outcome is analyzed over the number of selected trials and the resulting statistics generated. Furthermore, the distributive computing function prevents the creation of bins at the overall site level of resolution; thus, that series of comprehensive outputs can only be created running a complete simulation on a single machine.

Table 4-4. Model Trial Output Organization and Summary Statistical Bases

Site 216-X-001	Trial 1 Analyte Inventory Result	Trial 2 Analyte Inventory Result	Trial 3 Analyte Inventory Result	Trial 4 Analyte Inventory Result	Trial 5 Analyte Inventory Result	Results for Year Summation Bin (Fig. 4-1)
1961	a	h	o	v	ac	a,h,o,v,ac…
1962	b	i	p	w	ad	b,i,p,w,ad…
1963	c	j	q	x	ae	c,j,q,x,ae…
1964	d	k	r	y	af	d,k,r,y,af…
1965	e	l	s	z	ag	e,l,s,z,ag…
1966	f	m	t	aa	ah	f,m,t,aa,ah…
1967	g	n	u	ab	ai	g,n,u,ab,ai…
Results for Site Summation Bin	$T_1 = a + b + c + d + e + f + g$	$T_2 = h + i + j + k + l + m + n$	$T_3 = o + p + q + r + s + t + u$	$T_4 = v + w + x + y + z + aa + ab$	$T_5 = ac + ad + ae + af + ag + ah + aj$	$T_1, T_2, T_3, T_4, T_5, \ldots T_{25,000}$

During the simulation, **OCBHanford** creates the initial output reporting files as a function of the direction in the *Legend* worksheet in the production workbook. As the simulation progresses, the results are written to each output file and saved until the simulation completes. If an analyte, site, or operable unit was removed from the simulation, the resulting output file does not report it. Additionally, if there is an inadvertent interruption, SIM can be re-run and results obtained from the sites for which no calculations were performed and integrated with the pre-interruption results; however, this action will not correct the summary level statistical descriptions. If the summary level descriptions are necessary, a complete re-run is required.

The other executable files in SIM involve the distributive computation and reconstitution features, the post-process codes used to generate SAC output files, and data analysis treatments discussed in Section 5.0. These codes are written in visual basic for applications (VBA) and are executed at the user's direction.

4.1.3 Distributive Computation Features

Because of the size and run times associated with SIM, a simple distributed computing function was incorporated. The distributed computing management function was placed in the *Legend* worksheet of the production workbook. By placing an "X" or "x" in the appropriate column then executing the macro **OpUnit_Selection**, the corresponding sites of that Operable Unit are removed from the simulation. By using the **Update Operable Unit List and Split into Sections** macro, the computer will automatically load a file that is reasonably balanced as a function of the number of machines used to perform a simulation with the pieces having approximately concurrent run-time completions. These pieces are estimated using the number of site-year elements as a metric and are split into roughly equal numbers; however, sites within a specified operable unit are conserved (i.e., all members of an operable unit grouping are maintained together) within the same subfile. A simulation can be split among as many machines as is needed; however, the reconstitution function (**Merge** in the *Setup* worksheet) can handle a maximum of 10 files at a time.

4.2 COMPUTING INTERFACE AND INPUT SHEETS

There are three elements to the SIM computing interface. Two of them are part of the production workbook (*SIMInput_Base*) file—the *Setup* worksheet and the *Legend* worksheet; they are used to provide an interface for the user to define the boundaries and reporting requirements of the simulation.

The other interface element is the **OCBHanford** dialog box which activates the simulation. Once the parameters in the *SIMInput_Base* file are set, that specific file must be opened using **OCBHanford** as noted in Section 4.1.2, and the calculation executed. The calculation will then proceed as directed and outputs generated until the simulation is completed or interrupted.

4.2.1 *Setup* Spreadsheet

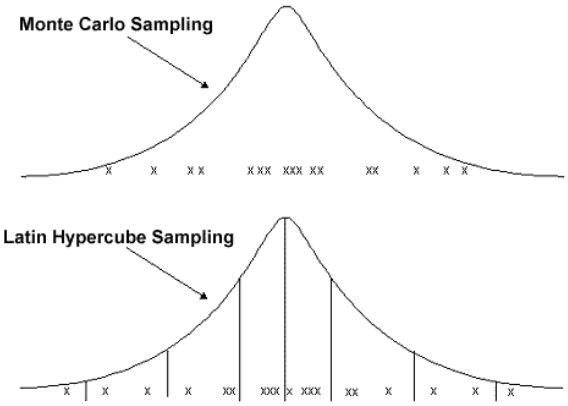
This is the top level administrative spreadsheet. The *Setup* spreadsheet is used to define, control, and report the Monte Carlo calculation parameters of SIM. These parameters are:

- Seed (Cell B4): This parameter is the random number seed. As part of the OCB kernel, if a seed value greater than zero is entered into this cell, the results will be exactly repeatable because a common random number list will be used. If the seed is zero, the random number generator will provide a similar result to a given model such that, with enough trials, the values will converge to whatever tolerance is desired, but the results will not be exactly repeatable.

- Trials (Cell B5): This is the number of times the model is simulated with random values for assumptions within the distribution definition. As discussed in Section 2.3, the number of trials needed to meet the desired convergence criteria in SIM was determined to be 25,000. Convergence analysis of the Monte Carlo output is addressed in Appendix B.

- Sampling Method (Cell B6): Open Crystal Ball® has two methods of simulation, Monte Carlo and Latin hypercube sampling (LHS). By setting this value to 0, a Monte Carlo calculation using a simple random sampling method will be performed. The random behavior in games of chance is similar to how the Monte Carlo simulation selects variable values at random throughout the selected probability distribution to simulate a model. In setting this value to 1, the LHS method will be selected. This sampling method works by segmenting the assumption's probability distribution into a number of non-overlapping intervals, each having equal probability, as shown in Figure 4-2. The LHS simulation can provide a faster convergence to a theoretical result than the simple random sampling Monte Carlo simulation for a given number of trials, because of the way in which the distribution is being sampled. However, demands on computing resources are higher for LHS (memory usage is higher and run-time performance is slower in the LHS simulation) and there is no guarantee of improvement (i.e., faster convergence).

Figure 4-2. Monte Carlo Sampling vs. Latin Hypercube Sampling



- LHS Sample Size (Cell B8): For the Latin hypercube simulation method, this value controls the number of interval segments and sample points across the segmented distribution for an assumption. Properties and impacts of bin size selection are discussed in Appendix B.

- Start/End/Duration (Cells B13 .. B15): This is the duration of the simulation. A calculated duration for the simulation using these start and end times is used, rather than the dynamic values reported in the Application Window. Additionally, this value is not a running total; thus, the total time will not be calculated unless the simulation completes.

- Create SAC Output (Cells A17…A20): The button, **Create SAC Output** activates a command that generates an output file that the SAC model can read and use in its computations. This output file is different in structure from the direct output files generated by SIM and does not contain the summary statistics for a site or operable unit, but contains the same site-year-analyte inventory and aggregate concentration and volume data.

- Percentiles (Cells G3 .. G23): There are twenty-one percentiles in a list. The number of percentiles reported must remain at twenty-one and are user defined. Percentiles are required for reporting the output to the FrcLiquid, FrcSolid, and FrcTotal spreadsheets. The percentiles may have varying intervals, but must be non-duplicate values from 0 through 100.

- Save Results Directory (Cell B26): This cell sets the pathname for saving the output from SIM.

- Notification (Cells B27, C27, and D27): These cells provide an e-mail address with subject line that can be notified as the simulation progresses, should a simulation require a long time to execute (e.g., greater than a workday) and the user desires a means of monitoring the progression of the simulation remotely.

- Optimization Parameters: Trials per loop (Cell B31): This cell defines the calculation size performed in one pass through the simulation. It must evenly divide into the number of trials and can be no greater than the number of trials.

- Combine Top 10 Lists: (Cell B35): This cell defines the pathway for recombining distributed models and creating a consolidated Top 10 list. Cells G34 to H36 define a button, **Merge Top 10 Lists**, for executing the command to initiate reconstitution of the distributed Top 10 lists into a single file.

- List the Resulting *SimInput* files (full location) to Merge into 'THIS' Empty Directory (Cells B39…B48): This merging macro uses the listed *SimInput* files to determine which set of distributed results are to be merged into the newly specified directory. A set of successful simulations are assumed to have occurred and that the various output files are located in the pathways specified with the above listed *SimInput* files. The macro, activated by the button Merge Summaries, begins execution at the top of the list and works its way down. The code uses the *Legend* sheet within the listed *SimInput* files to determine which Operable Units/Closure Zones were simulated and, therefore, the files to be merged to the newly specified directory.

4.2.2 *Legend* Spreadsheet

This spreadsheet is the backbone of the simulation. It defines the boundaries of the simulation—which sites, waste streams, and analytes that are to be included in calculating inventories in a simulation and it controls the distributed computing features in SIM. All input information is sorted and configured as defined in the *Legend* sheet. All of the data input sheets are directly related to the *Legend*. The *SiteInput* spreadsheet provides specific disposal volume data,

describing the waste site, year(s) of operation, and the waste stream(s) for both liquid and solids. The *AnalyteInput* spreadsheet defines the waste stream concentration data. *DensityInput* defines the density of a waste stream phase (solid or liquid).

The *Legend* matrices are also used to organize and report values to the output sheets. Input labels rather than identification numbers must be consistent from this page to the input spreadsheets. If there is an inconsistency (e.g., text vs. numeric values, inconsistent spelling or spacing, etc.) with the inputs during the attempted execution of the code, a dialog box will appear and describe what the problem is and where the problem is occurring within the workbook. There are three input matrices on this page:

- Waste Locations: The Waste Locations matrix provides the names for the sites that are used in organizing the input and output. This matrix assigns a unique numerical value, site name, and grouping assignment (currently by Operable Unit) to the locations to be calculated. Additionally, this section of the spreadsheet offers the ability to remove specific sites from the simulation. By placing an "X" or "x" in the appropriate column, the corresponding site will not be simulated. This feature was implemented for testing model performance to reduce simulations to a reasonable run-time, if a few select sites were of interest.

- Analytes/Radionuclides: The Analytes/Radionuclides matrix identifies the chemical species/isotopes being inventoried for the sites and assigns a unique numerical value, appropriate element/chemical name, and corresponding units in SIM. The unit assignments for each analyte/radionuclide are directly copied from these values to the output. Additionally, this section of the spreadsheet offers the ability to remove specific analytes from the simulation. By placing an "X" or "x" in the appropriate column, the corresponding analyte will be removed. This feature was implemented for testing model performance to reduce simulations to a reasonable run-time, if a few select analytes were of interest.

- Waste Stream: This matrix assigns a unique numerical value and name to each waste stream used in the simulation.

The matrices are not currently fixed in size in the modeling code. If there is a need to add locations, analytes, or waste streams to the model, they can be added to the current matrix, and included in SIM by maintaining the appropriate identification number sequence and labeling. Similarly, if a parameter needs to be deleted, that change can be accommodated as well. However, there cannot be any blank cells in the input matrices because the modeling code determines the maximum number of sites, analytes, and waste streams in each matrix by stepping through the array until it finds an undefined cell. Thus, the elements of these matrices must be contiguous and the identification numbers must be sequential integers for the model code to execute. Cells containing a space, ' ', within a label are not considered "undefined" cells, but may interrupt the model execution because of the potential ambiguity. If this error occurs, the model will describe the problem and its location to the user within the workbook in a message box.

5.0 SIM OUTPUT DESCRIPTION AND ORGANIZATION

This section describes the various outputs from SIM. Each of these outputs is used in either providing the requested results to SAC, or as tools for internal technical review and analyses. The overall format of the general model follows the logic and nomenclature seen in Figure 5-1. The results from this modeling effort provide a wide range of inventory information beyond the mean and standard deviation. The percentile data necessary to construct a complete (albeit coarse) probability distribution function (pdf) are collected for each analyte. This information is necessary to provide the required modeling input information to the SAC. It also aids in interpreting the data, allowing an analyst or reviewer to see the shape of the output. In addition, inventory results for each waste site as a function of time, location, and phase, is included in the summary results.

5.1 MODEL RESULTS

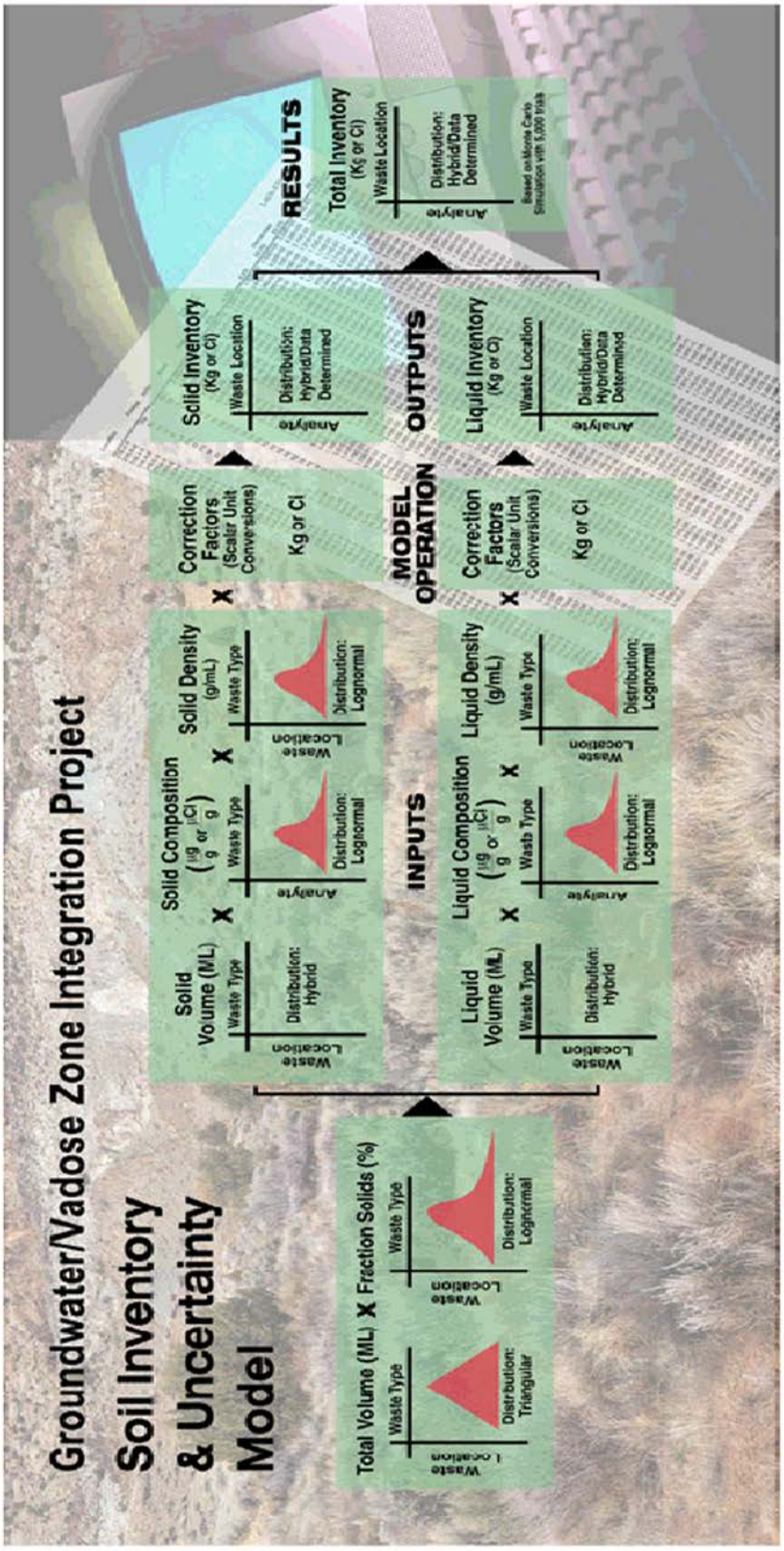
There are two types of results generated by SIM: direct outputs and verification/analysis outputs. The outputs described in this section are the file outputs generated directly by **OCBHanford** and its associated production codes. Section 5.1.1 describes the separate output workbooks containing the results organized by operable unit. Section 5.1.2 describes the SAC Output files created by the production macro. Section 5.1.3 describes the *SumFrc* spreadsheets in the *SimInput_Base* file. Section 5.1.4 describes the *Top 10 list*.

5.1.1 Results by Operable Unit Workbooks

The comprehensive SIM outputs are reported in separate workbooks organized by operable unit (200-E Ponds Zone, 200-W Ponds Zone, B Farm Zone, B Plant Zone, NRDWL-BC Control Zone, PFP Zone, PUREX Zone, REDOX Zone, S-U Farm Zone, Semiworks Zone, Solid Waste Zone, T Farm Zone, T Plant Zone, U Plant Zone, Unassigned 200 Area Zone [three separately reported], Unassigned 300 Area Zone, WM Zone, and WTP-ETF-A-C Farm Zone). The site grouping organization can be constructed using any number of desired criteria; however, care must be taken to ensure that no output file exceeds the maximum length of an Excel worksheet (65,536 rows); otherwise, the computation will cause the computer to stall, and the code will not run to completion.

Each site-year-analyte-phase combination inventory result is reported along with total inventory results for each analyte by site and the comprehensive total for the operable unit. In addition, the input volume is described in terms of percentiles in order to derive a corresponding concentration percentile value for the site-year-analyte combination. Therefore, these concentration and volume percentile data are also calculated and are provided in the individual operable unit/closure zone results workbooks.

Figure 5-1. General Soil Inventory Model Architecture



5.1.2 SAC Output Files

The current SIM outputs and consolidated results are useful in a variety of ways, from diagnosing systemic errors in modeling to evaluating specific site-year analyte results of interest. However, the Inventory Module used in SAC (Bryce et al. 2002) to evaluate groundwater contamination requires the SIM-generated inventories to be decoupled into concentration and volume components to be used as inputs. These components are generated concurrently and reported together with the inventories providing a comprehensive, consolidated quantitative description of the site-year analyte inventories. The **Create SAC Output** macro takes the specified set of output files in a directory and assembles them into a structure that can be directly read by SAC. Some post-processing of these files is necessary to accommodate client hardware, software, and electronic transmittal constraints because they are large and unwieldy files (~350 MB).

5.1.3 Summary *SumFrc* Spreadsheets (SumFrc Total, SumFrc Liquid, and SumFrc Solid)

These summary spreadsheets are part of the *SimInput_Base* file. They provide the total inventory by operable unit and the total site inventory (as a summary of the summations for each operable unit). As noted previously, the comprehensive site inventory summary results are not available if a distributed model is performed because the overall binning information is not carried over in that process. The labels are relatively self-explanatory: *SumFrc Total* (summary, fraction total), *SumFrc Liquid* (summary, fraction liquid), and *SumFrc Solid* (summary, fraction solid). These results provide measures of central tendency and uncertainties for consolidated groupings that are useful for evaluating global inventories. The partition of inventory by phase is useful in further evaluating waste stream and site characteristics.

5.1.4 *Top 10 Lists* Spreadsheets

The ***Top 10 lists*** are diagnostic tools and offer a high-level view of the overall model results. Its function is also self-explanatory—the ***Top 10 list*** provides a list of the site locations for the 10 highest total inventory and concentration values for each analyte. The values measured are mean inventory, median inventory, and RSD at the consolidated site level. This series of results provides where the largest inventories for a particular analyte are and where the most uncertain inventory values are. From a diagnostic standpoint, this table allows for evaluation of significant systemic errors or patterns in the input. From an overall view of the model results, the selected organization of the results is an efficient method for inspecting and evaluating the data. These data are necessary to determine specific site risk and application of potential mitigation strategies and resources.

5.2 VERIFICATION/ANALYSIS OUTPUTS

The outputs described in this section are the data verification and analysis outputs generated by the post-process VBA codes that are part of the production workbook. These elements are not part of SIM directly (i.e., they are not part of the inventory quantification calculation), but are necessary components for SIM and its outputs to function and be useful. Section 5.2.1 describes the *cCDIDatabaseQuery* worksheet; Section 5.2.2 describes the *0,1,2 compare* worksheet; Section 5.2.3 describes the *cCDIPu239, cCDISr90, cCDICs137, cCDIU238* comparison and *lessthans* worksheets; Section 5.2.4 describes the *SiteEval* worksheet; Section 5.2.5 describes the *VolumeBalance* worksheet; and Section 5.2.6 describes the *Blackboxtest1* worksheet.

5.2.1 Consolidated Site Reference Database (*cCDIDatabaseQuery* Worksheet)

This worksheet assembles the specific SIM-Diediker site/analyte comparisons (e.g., individual 2^{nd} order results) and evaluations for the selected analytes. It provides a rollup of the individual Cumulative Database Inventory (CDI) comparison results that feeds the *0,1,2 compare* worksheet, as well as quantifies SIM performance on a site-specific basis. This worksheet is also where the impact of "less than" inventory values are incorporated. Cells colored blue are the "less than" values included in Diediker (1999); cells colored light green are the "less than" values found in other source documents that were not carried forward as "less than" values to Diediker. Other cells, shaded yellow, highlight corrections to the supplied data that were incorporated as part of this comparison.

5.2.2 Model Granularity Comparison (*0,1,2 Compare* Worksheet)

This worksheet presents the 0^{th}, 1^{st}, and 2^{nd} order comparison results for SIM. Zeroth order comparison results are presented as a function of comprehensive radionuclide losses as compared to the ORIGEN2 production information and individual analyte losses for Pu-239, U-238, Cs-137, and Sr-90 summed up over disposal locations in the 200 Areas as a whole. Each operable unit/closure zone is presented with its consolidated inventory estimates for individual analytes as well as in a combined 0^{th} and 1^{st} order results table to illustrate the model performance at those levels. However, the comparisons require a one to one correspondence for the comparisons to be valid. Thus, a site that does not have an inventory estimate from Diediker (1999) for one of the analytes is excluded from this evaluation and the quantitative comparison. In addition, the combined 2^{nd} order model comparisons for each of the four analytes are presented with the stage-wise impacts of the "less than" values on the results.

5.2.3 Specific Analyte Comparison (*cCDI Analyte Comparison* and *Lessthan* Worksheets)

Each of the specific analyte comparison worksheets are structured the same: the overall inventory range calculated by SIM for each of the analytes is stored in these worksheets by percentile as well as the Diediker inventory value. Indices from SIM are matched to the same sites and analytes found in Diediker (1999) to enable comprehensive automated data comparisons via a macro command and to aid in further data analysis. As part of the analysis, an evaluation of the cCDI (compare Cumulative Decayed Inventory) value within the range of

model estimates is performed. If a cCDI value is anywhere within the SIM range of values, that outcome is considered agreement between the SIM result and the Diediker database (e.g., result "in range"), and is assigned a value of "1" for use in further data analysis and evaluation. If the SIM range of values is consistently higher than the CDI value and does not encompass it, that outcome is considered disagreement between the SIM result and the Diediker database (e.g., result "SIM high"), and is assigned a value of ".001" for use in further data analysis and evaluation. If the SIM range of values is consistently lower than the CDI value and does not encompass it, that outcome is considered disagreement between the SIM result and the Diediker database (e.g., result "SIM low"), and is assigned a value of "1000" for use in further data analysis and evaluation. These quantitative assignments of SIM versus reference data performance are then carried forward and further evaluated and consolidated during data processing and analysis.

Additionally, there is a worksheet that contains reference values that are quantified as "less thans" (called *lessthan).* This worksheet contains the cell locations and category of "less than" values used in Diediker (1999) or other reference documents. The calculation that determines model performance (e.g., CDI value inside or out of range) references this set of cells to adjust for the impact of these values on the comparisons made. If the SIM results estimated are consistently less than the CDI or other reference "less than" value, a correction to the performance evaluation comparisons are made and credit for that site-analyte combination is given in the SIM evaluation comparison. The impact of these "less than" values on SIM performance is then tracked on the *0,1,2 compare* worksheet. Furthermore, there have been corrections to the Diediker database values where inspection of the source data has revealed a discrepancy. The corrections have been incorporated and documented as part of Table 6-32 in Section 6.0.

5.2.4 Site Eval (Site Evaluation) Worksheet

The *Site Eval* spreadsheet is a diagnostic tool that allows investigation of a specific analyte inventory at a particular site in the *Top 10 list*. On activation of the **Top10_Eval** macro, the *Site Evaluation* worksheet will be populated with the model input parameters and uncertainty definitions for that site-analyte combination and run a conventional Crystal Ball 2000® Monte Carlo scenario so that the individual contributing elements to the total inventory can be evaluated. However, the *Site Evaluation* spreadsheet can only run one site-analyte combination at a time on the *Top 10 list*, although multiple evaluation scenarios could be saved in a separate workbook if the user desired.

5.2.5 *VolumeBalance* Worksheet

The *VolumeBalance* worksheet provides a compact way of reviewing the total volumes of waste discharged in three ways: by waste stream as a function of time; by year, with each total waste stream contribution, and by total waste stream volume. Thus, waste losses can be reconciled and allocated to the proper time and amount. This worksheet aids in enforcing the overall mass balance boundary condition and can assist in evaluating analyte solubilities and volume percent solids lost.

5.2.6 *BlackBoxtest1* Worksheet

The *BlackBoxtest1* worksheet performs an independent test of the OCB results by running the *Top 10 list* outputs for RSD results comprehensively through the **Top10_Eval** macro and compares those results to the output obtained using regular Crystal Ball. This test is done as an internal QA consistency check to establish that the model parameters and computation commands are functioning correctly, the calculations are being performed correctly, and as a second check on satisfying the convergence criteria.

6.0 RESULTS AND DISCUSSION

Each waste site location or tank leak has the same set of chemicals and radionuclides reported. The mean, standard deviation of the mean, and the median are reported as well as the percentiles defining the probability distribution function (pdf) for 99% of the area for the output distributions. The electronic attachments contain the SIM input components and outputs. Appendix A contains the waste stream input derivation data, waste site description and more detailed discussion regarding the derived modeling assumptions. Appendix B contains a description of the quality assurance protocols and summarizes the results from the model quality assurance trials. Appendix C is an electronic only file and contains the production results organized by operable unit. Appendix D is an electronic only file and contains the production input definitions and WSWB.

For purposes of this analysis, the focus of discussion will center on nine of ten analytes selected by SAC in their inventory evaluation, with specific emphasis on four analytes. These specific analytes are Pu-239, U-238, Cs-137, Sr-90; the remaining analytes to be evaluated are Tc-99, H-3, I-129, U-Total, CCl_4, and Cr. U-Total and U-238 are alternately reported and compared, depending on the reference data basis (most reference data presents uranium as U-Total in kilograms, rather than segregating each isotope by Curies). However, a broader discussion of inventory and uncertainty will be presented for various analytes in selected cases.

In the simplest modeling case, a zero-order model would be strictly a function of volume received because that simple model would assume that the waste received by a particular site was indistinguishable from site to site. By inspection of the data and from documented knowledge of the waste management practices at the Hanford Site, this condition is known not to be true for the wastes disposed to the vadose zone (e.g., the waste inventories disposed were dependent on time and location). Therefore, in this case, the n^{th} order model condition was defined as corresponding to the amounts of waste (analyte inventories) disposed to the entire 200 Area (0^{th} order), the various Operable Unit/Closure Zones (1^{st} order), and the specific site within a closure zone (2^{nd} order), and for the purposes of evaluation, the model results were categorized and compared by the level of resolution of the results. Table 6-1 provides a list of sites with their volumes and the percent of total volume received. This quantification provides a benchmark for comparison when other site inventories are evaluated.

Table 6-1. Top 10 200 Area Sites by Volume Received. (2 Sheets)

Site	Mean Volume (ML)	Percent of Total Mean Volume in SIM
216-A-25	2.94E+05	28.72%
216-B-3	2.83E+05	27.63%
216-U-10	1.60E+05	15.62%
216-T-4A	4.28E+04	4.19%
216-S-16P	4.07E+04	3.98%
216-B-63	7.98E+03	0.78%

Table 6-1. Top 10 200 Area Sites by Volume Received. (2 Sheets)

Site	Mean Volume (ML)	Percent of Total Mean Volume in SIM
216-A-30	7.64E+03	0.75%
216-S-10 and S-11 System	6.73E+03	0.66%
216-S-17	6.44E+03	0.63%
216-U-14	4.88E+03	0.48%
Top 10 Total	8.54E+05	83.42%

6.1 SITE CATEGORY INVENTORY EVALUATION

Evaluating the model results from a strictly volumetric point of view, the disposal sites contribute the vast majority to the inventory lost to the ground. And on further inspection, the degree of correlation between volume and total inventory is quite close for several analytes. However, for some others, there is a significant tilt towards the much smaller, but much more concentrated inventory sources (tank and unplanned release losses). Figures 6-1 to 6-9 illustrate the percent contributions of the various analytes to inventory by loss category (e.g., disposal site, tank leak, or unplanned release) as a percentage disposed or released. Figure 6-10 illustrates the volumetric breakdown by category. In the following charts, contributions less than 1% are rounded down to zero.

Figure 6-1. Tritium Inventory Contribution by Site Category

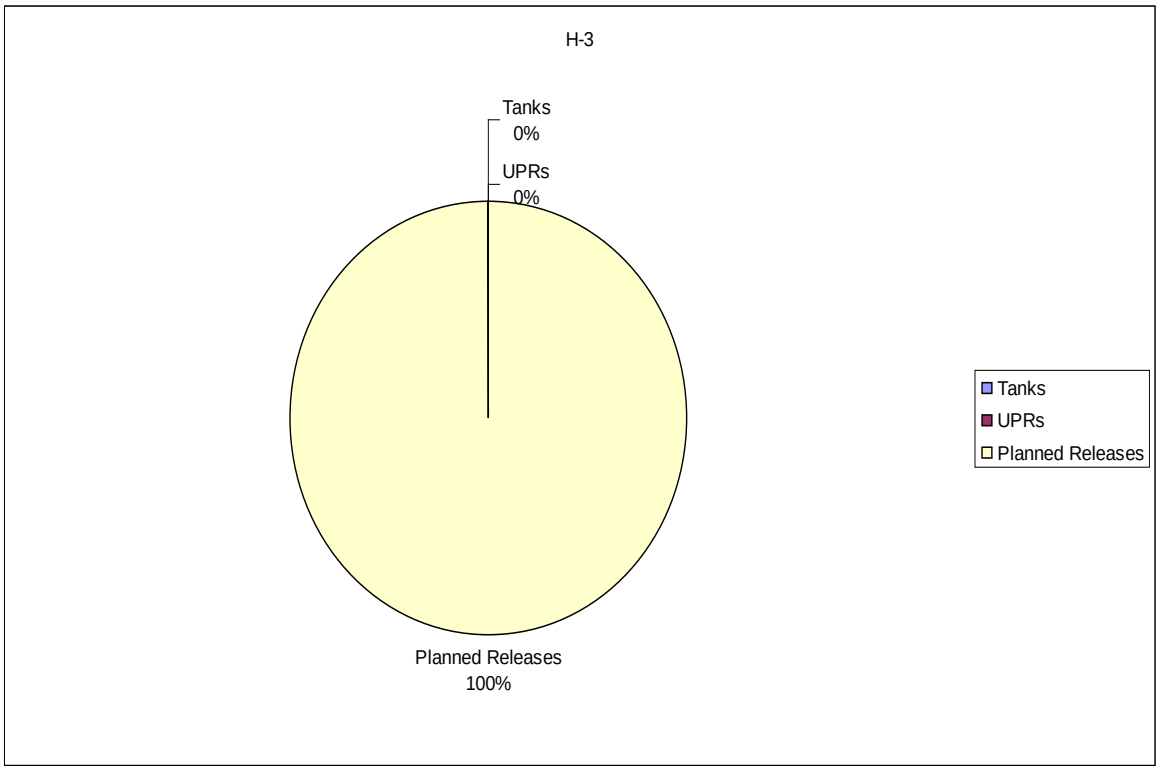


Figure 6-2. Tc-99 Inventory Contribution by Site Category

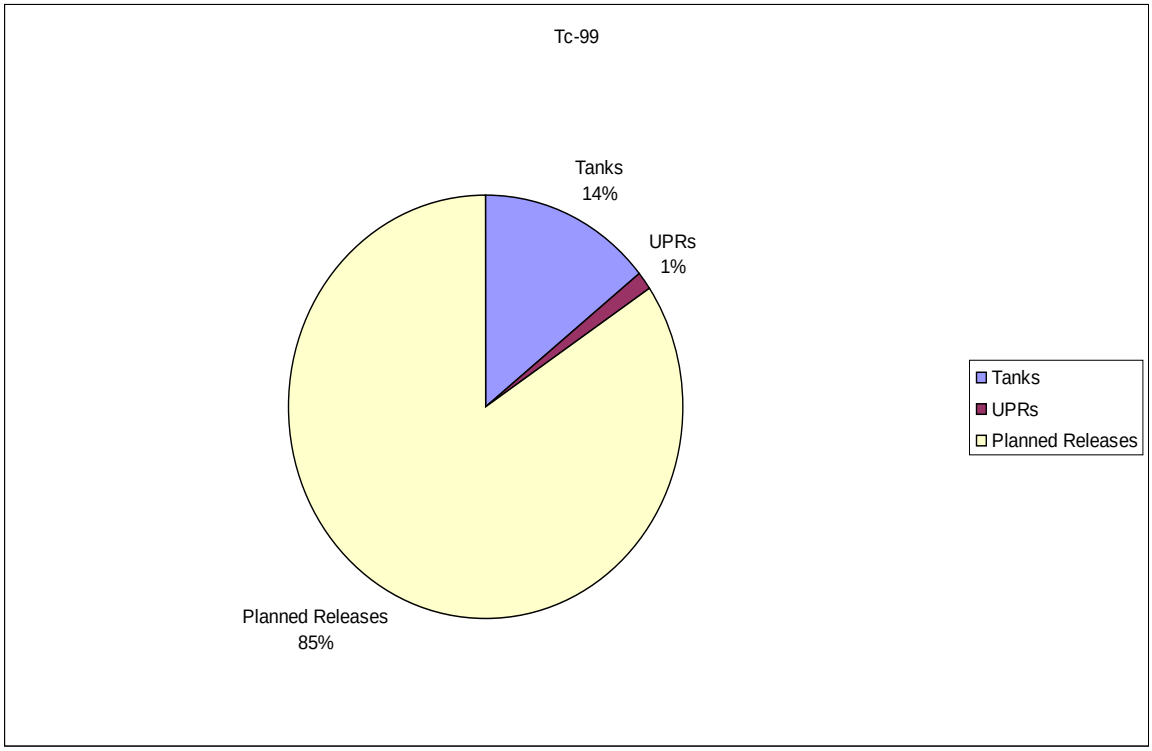


Figure 6-3. I-129 Inventory Contribution by Site Category

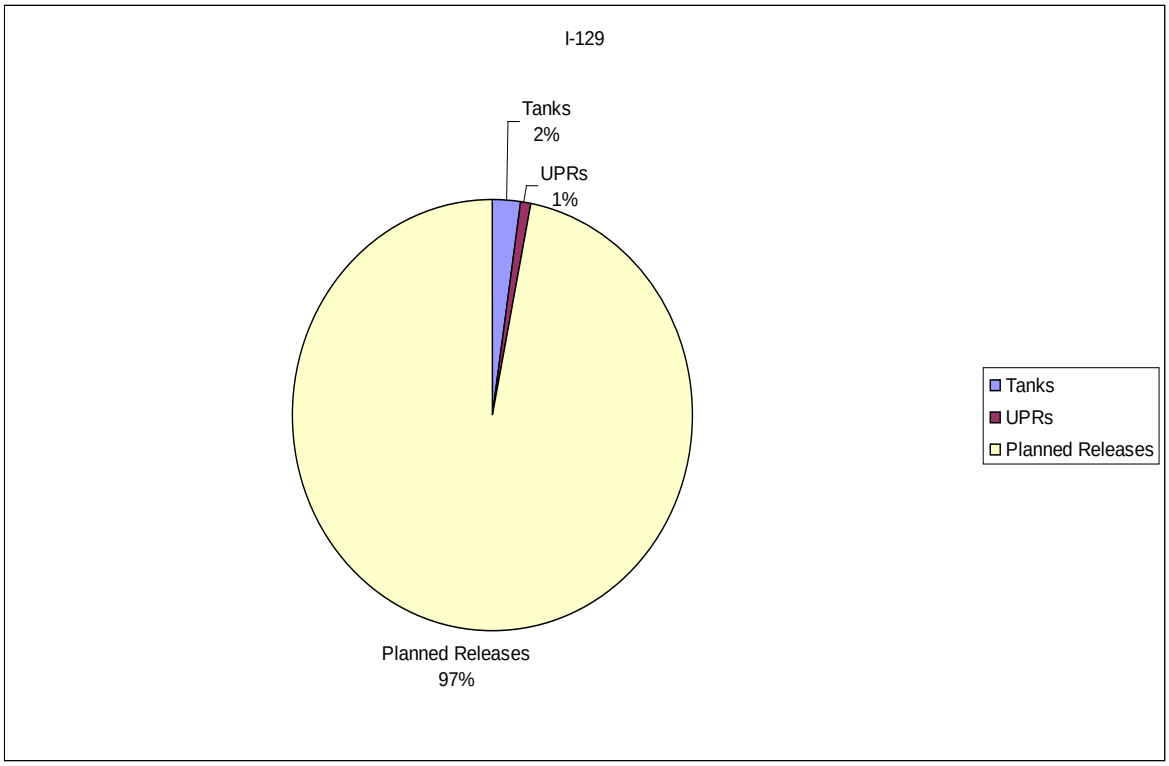


Figure 6-4. Cs-137 Inventory Contribution by Site Category

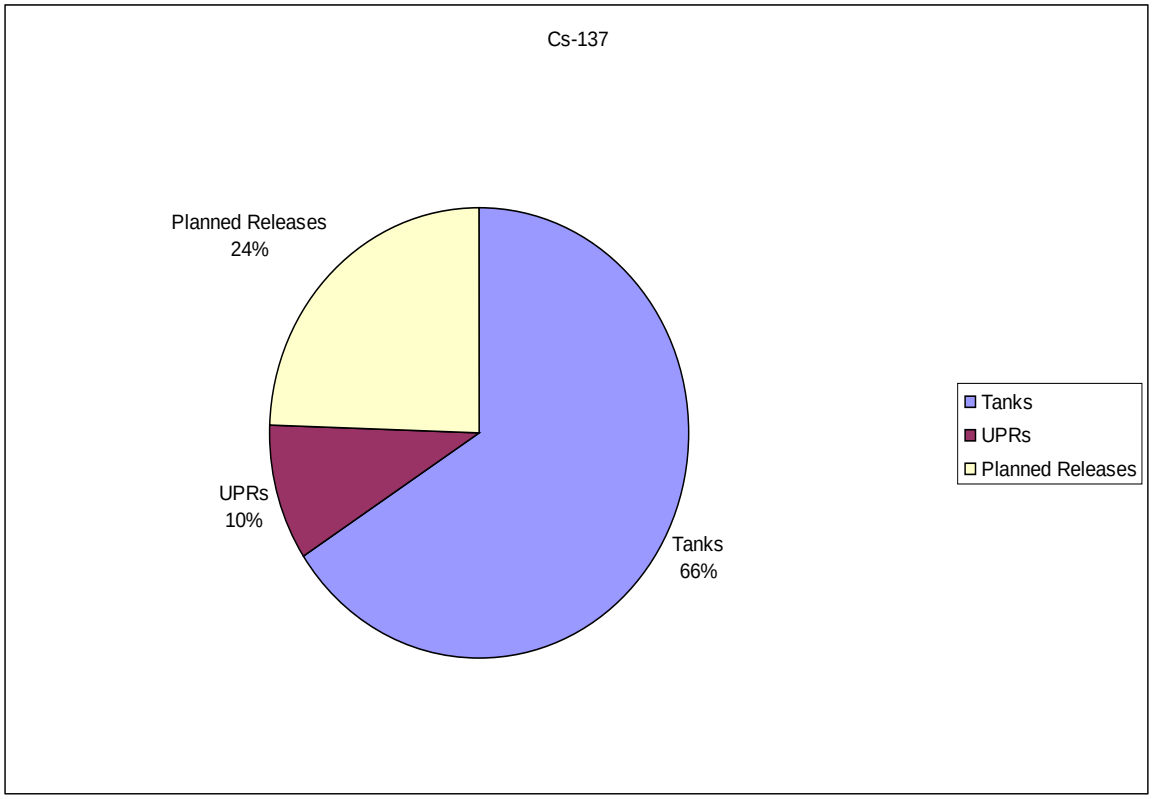


Figure 6-5. Sr-90 Inventory Contribution by Site Category

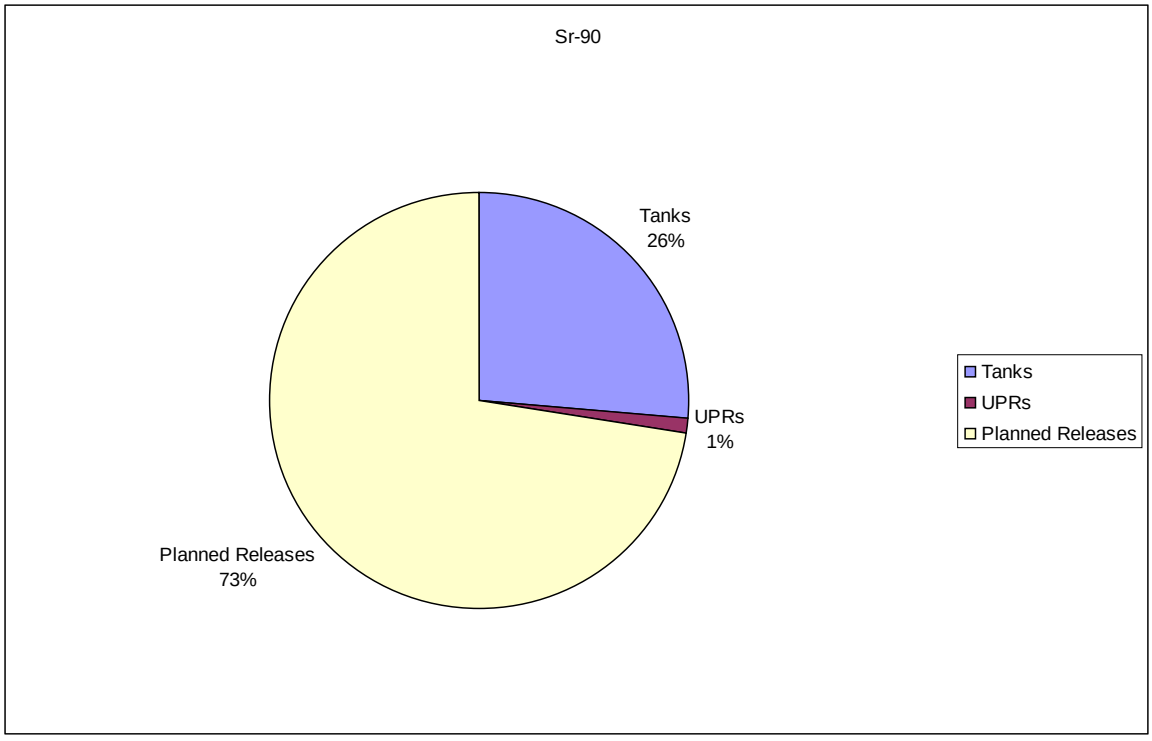


Figure 6-6. Uranium Inventory Contribution by Site Category

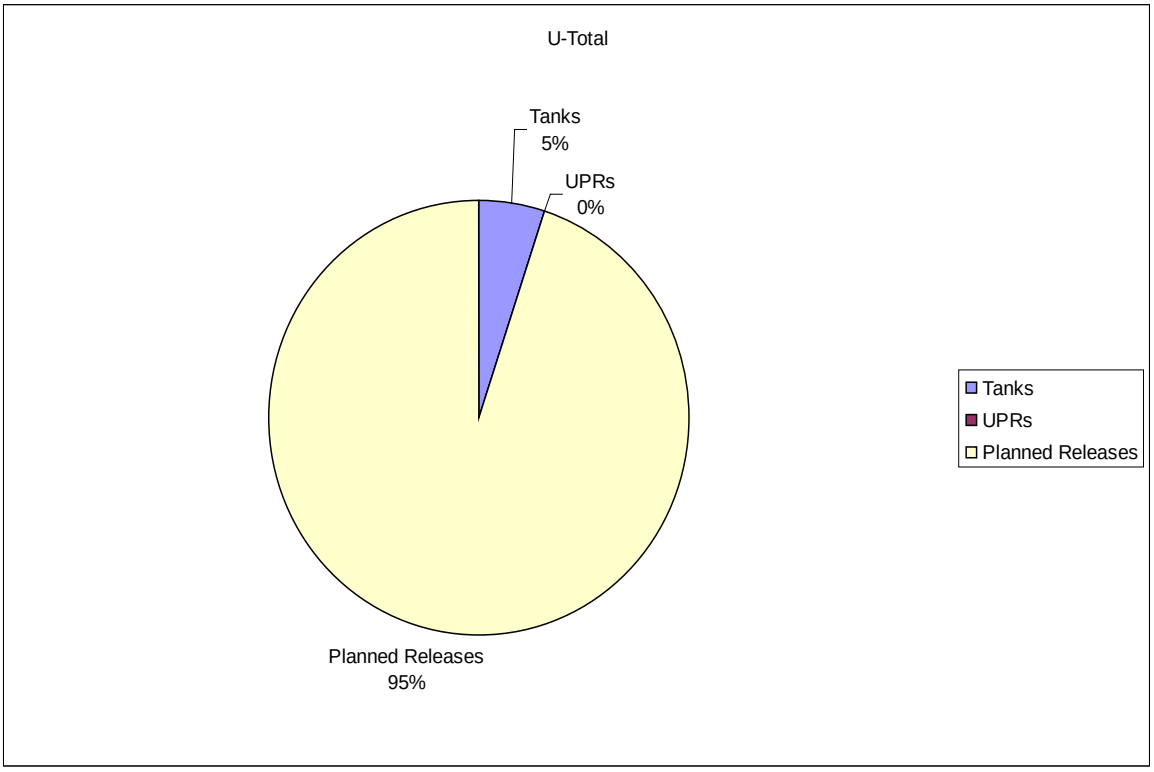


Figure 6-7. Pu-239 Inventory Contribution by Site Category

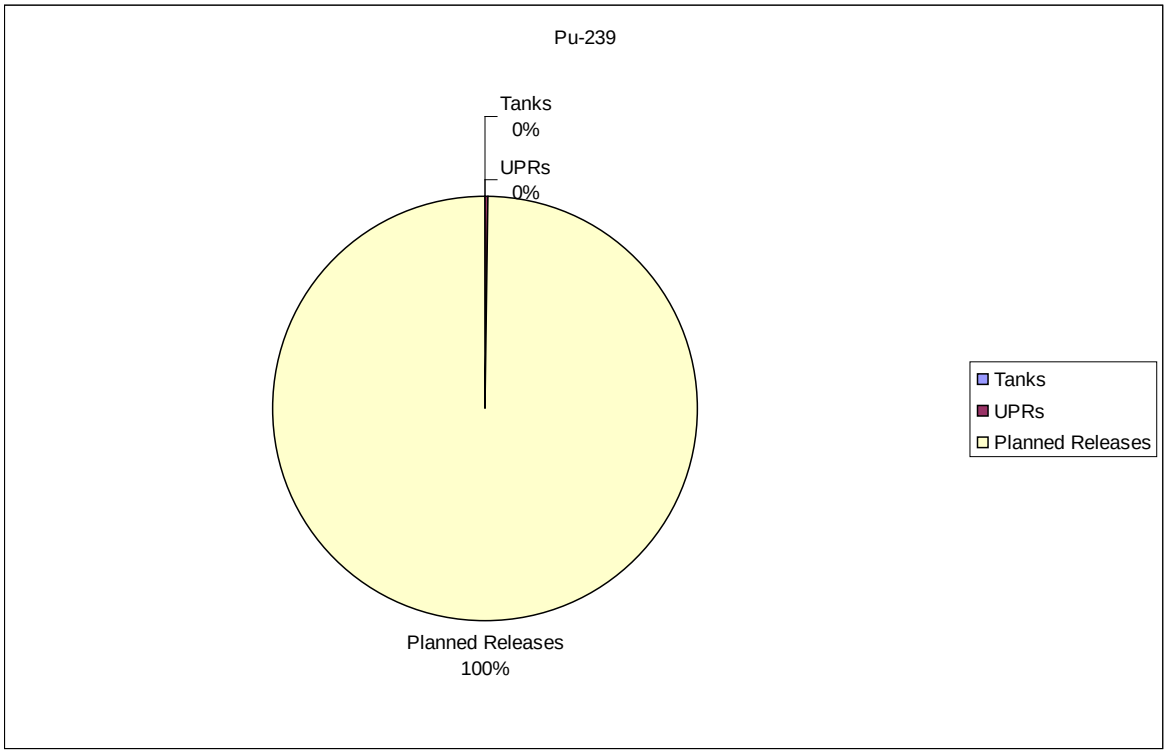


Figure 6-8. Carbon tetrachloride Inventory Contribution by Site Category

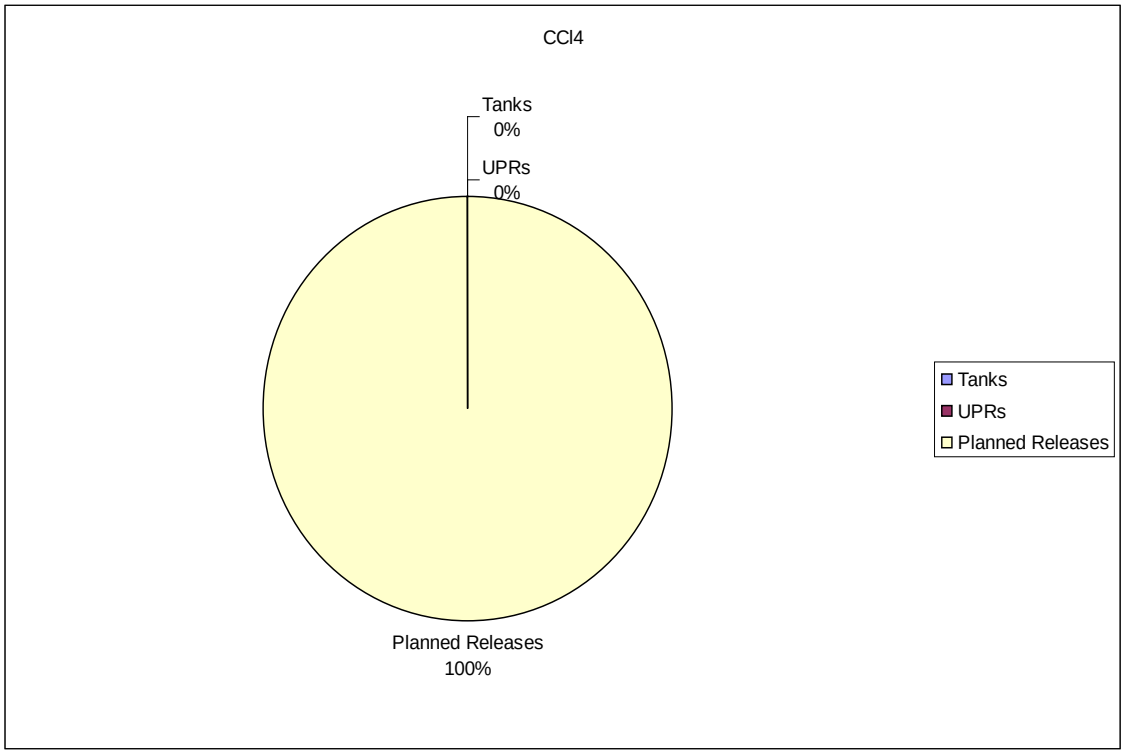


Figure 6-9. Chromium Inventory Contribution by Site Category

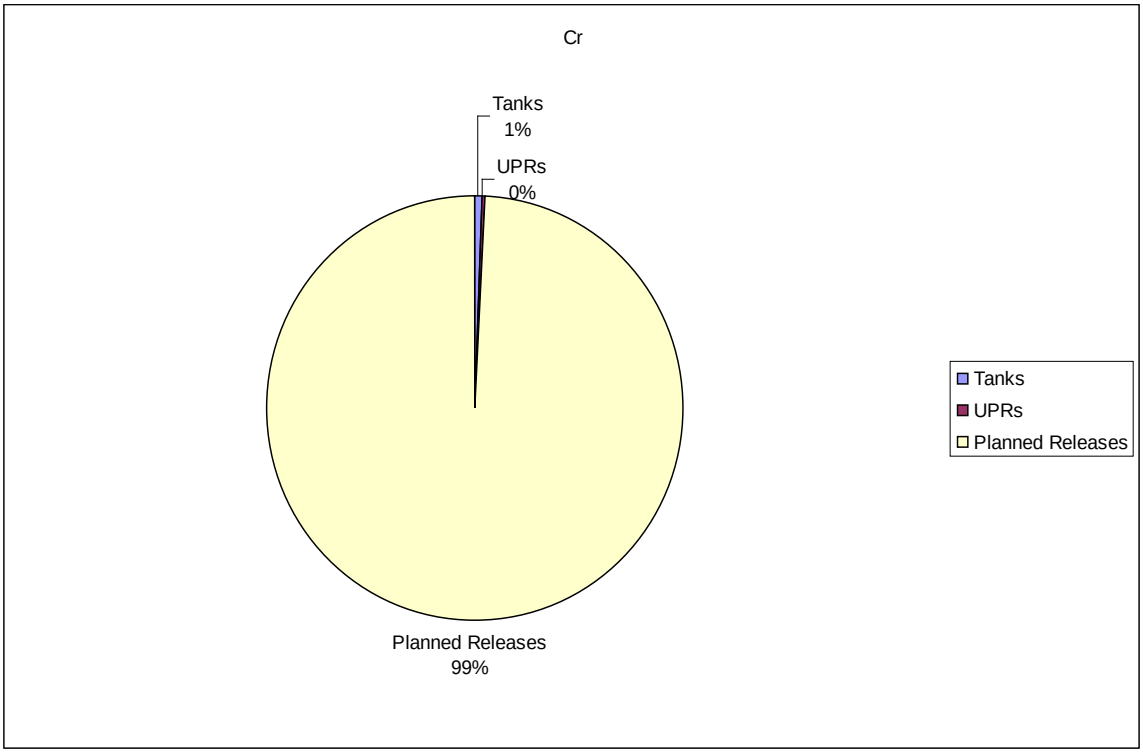
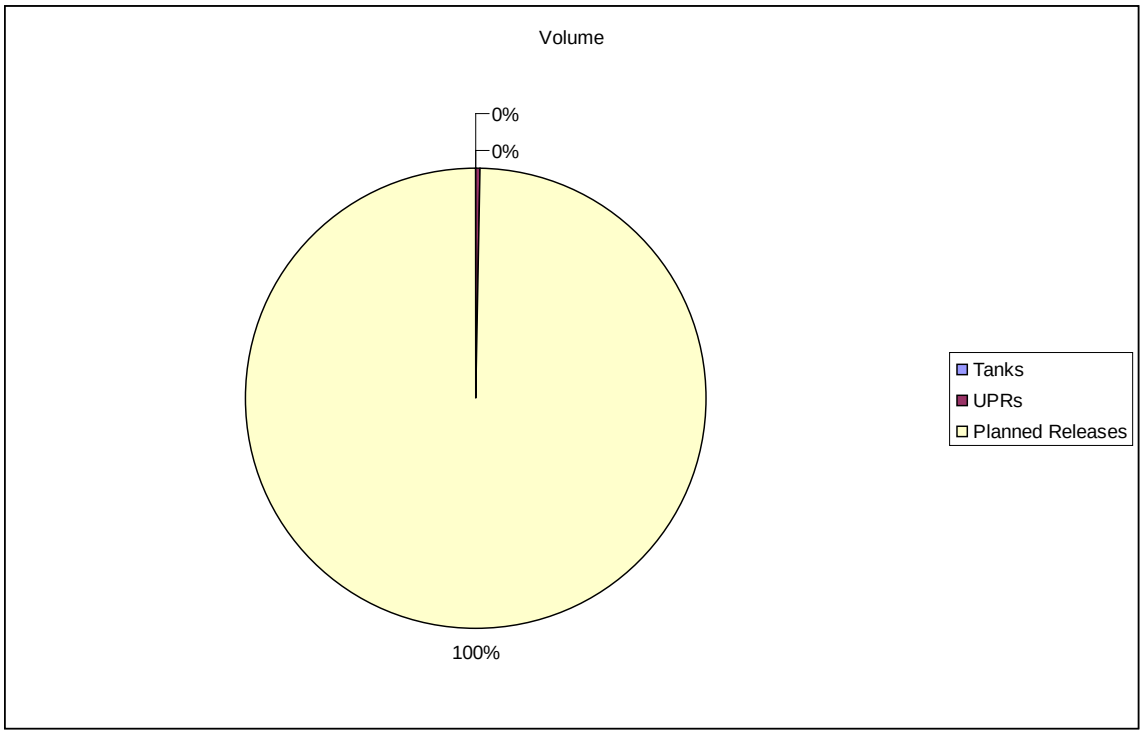


Figure 6-10. Volume Disposed or Released by Site Category (as a percent)



6.2 ZERO-ORDER AND FIRST-ORDER INVENTORY COMPARISONS—ANALYTES FOR THE 200 AREA PLATEAU

There are a few relevant comparisons that can be made at the zero order (site wide) level—the comparisons that will be presented in the following section consist of comparing the amount of radionuclides generated from ORIGEN2 estimates to the overall totals estimated discharged to the vadose zone. Additionally, for the four selected analytes, determining the resulting overall documented vadose zone inventories within the context of the SIM estimated values and quantified uncertainty is also shown.

6.2.1 Zero-Order Comparisons—SAC Selected Analytes, Site-wide

Table 6-2 illustrates the inventory totals for the selected SAC analytes for the overall inventories computed for the waste sites and how they compare with the mean estimated production inventories calculated from ORIGEN2. A 1% to 2% loss from the tank-canyon system was expected for the separations plants. Where reprocessing and recycling streams were involved, it was anticipated to be higher. For all results presented, the values are for the combined solid and liquid inventories unless otherwise specified.

Table 6-2. SIM Analyte Inventory Totals (Decayed to 1/1/2001). (2 Sheets)

Radionuclide	ORIGEN2 Total	SIM Mean Totals for All Sites	SIM Value as a % of Total
H-3 (Ci)	1.85E+05	1.77E+05	95.68%
C-14 (Ci)	3.94E+03	1.97E+02	5.00%
Ni-59 (Ci)	1.33E+03	8.24E+00	0.62%
Ni-63 (Ci)	1.27E+05	8.06E+02	0.64%
Co-60 (Ci)	1.61E+04	8.64E+01	0.54%
Se-79 (Ci)	7.90E+01	2.15E+00	2.72%
Sr-90 (Ci)	8.79E+07	5.15E+04	0.06%
Y-90 (Ci)	8.79E+07	5.15E+04	0.06%
Zr-93 (Ci)	4.72E+03	8.47E+01	1.79%
Nb-93m (Ci)	3.73E+03	7.16E+01	1.92%
Tc-99 (Ci)	3.43E+04	6.87E+02	2.01%
Ru-106 (Ci)	1.06E+03	3.58E-02	0.00%
Cd-113m (Ci)	5.79E+03	7.63E+01	1.32%
Sb-125 (Ci)	1.90E+04	7.37E+00	0.04%
Sn-126 (Ci)	3.29E+02	7.86E+00	2.39%
I-129 (Ci)	4.94E+01	4.72E+00	9.56%
Cs-134 (Ci)	8.56E+03	1.82E-01	0.00%
Cs-137 (Ci)	1.04E+08	2.23E+05	0.21%
Ba-137m (Ci)	9.83E+07	2.10E+05	0.21%
Sm-151 (Ci)	3.30E+06	8.53E+04	2.58%
Eu-152 (Ci)	1.07E+03	4.67E+00	0.44%
Eu-154 (Ci)	9.19E+04	3.58E+02	0.39%
Eu-155 (Ci)	5.14E+04	1.95E+02	0.38%
Ra-226 (Ci)	1.76E-02	1.02E-02	57.80%
Ra-228 (Ci)	3.04E+00	7.34E-03	0.24%
Ac-227 (Ci)	4.66E+00	5.05E-02	1.08%
Pa-231 (Ci)	7.15E+00	9.35E-02	1.31%
Th-229 (Ci)	1.41E+00	3.59E-04	0.03%
Th-232 (Ci)	2.80E+00	4.24E-04	0.02%
U-232 (Ci)	7.48E+00	2.27E+00	30.40%
U-233 (Ci)	4.49E+02	1.36E+02	30.19%
U-234 (Ci)	2.69E+03	7.21E+01	2.68%
U-235 (Ci)	1.20E+02	3.06E+00	2.56%
U-236 (Ci)	3.53E+01	1.60E+00	4.52%
U-238 (Ci)	2.72E+03	6.88E+01	2.53%
U-Total (kg)	8.15E+06	2.06E+05	2.53%
Np-237 (Ci)	1.32E+02	5.36E+01	40.51%
Pu-238 (Ci)	1.98E+03	7.23E+02	36.45%
Pu-239 (Ci)	3.37E+04	1.18E+04	34.96%
Pu-240 (Ci)	8.11E+03	2.90E+03	35.83%
Pu-241 (Ci)	1.27E+05	3.75E+04	29.45%
Pu-242 (Ci)	7.94E-01	3.27E-01	41.17%
Am-241 (Ci)	8.27E+04	2.87E+04	34.71%
Am-243 (Ci)	4.22E+01	1.15E+01	27.26%

Table 6-2. SIM Analyte Inventory Totals (Decayed to 1/1/2001). (2 Sheets)

Radionuclide	ORIGEN2 Total	SIM Mean Totals for All Sites	SIM Value as a % of Total
Cm-242 (Ci)	7.33E+01	1.99E+01	27.13%
Cm-243 (Ci)	7.74E+00	1.42E+00	18.32%
Cm-244 (Ci)	1.92E+02	3.44E+01	17.98%

Except for tritium, which may be expected to contribute a substantial fraction of its overall production to the vadose zone because of its complete miscibility in water and high volatility (e.g., it will be found in tank and process condensates), the relative total loss amounts of most these analytes are small (less than 5%) compared to the production inventories. This performance demonstrates that the waste management activities in place at the Hanford Site over its history performed reasonably well, and that most of the radionuclides are believed to be contained within the tank-canyon system.

Many of the analyte loss amounts are much less than anticipated. In most of these cases, these analytes have characteristics that make their unexpectedly low loss ratio more reasonable.

- Rapid decay—certain radionuclides such as Ni-59, Co-60, Ru-106, Cs-134, and europium have relatively short half-lives in comparison to most of the other radioisotopes and so their loss ratios do not necessarily scale or behave as anticipated.

- Production timing—there is almost no loss of certain isotopes because of peculiarities of timing; for example, thorium isotopes from the tank-canyon system. The overwhelming majority of these residual analytes remain in the tanks, and where there are losses, they are the result of tank leaks and unplanned releases. The reason for this behavior is that these particular isotopes were produced and extracted in quantity at two very specific times, 1966 and 1970. Most of the sites under examination in SIM did not receive high-level process wastes past 1960 and direct discharge of process wastes to cribs was substantially reduced as a waste management practice from the mid-1960s forward. Those sites that remained in active service past the mid-1960s generally received non-contact waste streams that did not have much contamination.

- Reclamation/recycling—because of the various efforts to extract cesium and strontium from the waste tanks to reduce heat load and for possible isotope commercialization, Cs-137 and Sr-90 are significantly impacted by this characteristic and their loss ratios are much lower (although, in the case of plutonium, this characteristic interacted with some other parameters and the loss ratio was higher than anticipated). Also, because these analytes were relatively easy to detect, these fission products were often used as tracers for surveillance alarms or as the limiting factors in disposal inventory.

However, there are several notable results (analytes with losses greater than 5%) that require some additional discussion.

Iodine-129 is high as a result of using environmental surveillance data to calibrate I-129 losses to the ground (Kincaid 2004; Appendix A). Radium-226 is high because of a modeling artifact with regard to how the ORIGEN2 data calculated that quantity for the timeframe of interest (the early bismuth phosphate processing era) and the association of this analyte with the disposal of ferrocyanide wastes to the ground. The losses of certain uranium isotopes, U-232 and U-233, are elevated for similar reasons—the ORIGEN2 source term calculations and timeframes involved for defining the fuel fabrication waste streams in the 300 Area are particularly high in concentration for these isotopes and the site description indicates that a modest amount of waste solids ought to be present.

The losses for the actinide components in general are elevated because these results are the product of fundamentally different processes and source terms from a modeling perspective. In this case, the purified plutonium product streams and scrap recycle streams represent a different source term from the fission products being evaluated. These analytes were concentrated and accumulated in Z Plant and, thus, are not necessarily related directly to the fuel processing time or separation plant like the other waste streams. In addition, the ORIGEN2 total results represent a decayed and extracted source term. Therefore, these losses represent a substantially larger proportion for these analytes (e.g., the baseline ORIGEN2 values are the residues of these analytes remaining at Tank Farms).

Another relevant comparison is to see if the resulting overall inventory estimates correspond to accepted literature estimates. For this comparison, a 99% estimate range for each analyte was selected as the basis for comparison. This comparison only incorporates data from where there is an accepted literature value in Diediker (1999) that was not determined to be in dispute with other historical information. The complete comparison is discussed in further detail in Section 6.3. However, at the zero-order level, Table 6-3 illustrates how the mean model values and the high and low percentile values compare with the literature data for a corresponding data set.

Table 6-3. Zero Order Comparison—Comparison for Four Analytes for Selected 200 Area Sites (Cs-137, Sr-90, U-Total, Pu-239)

Zero Order Comparison	Sum of Mean SIM values	Sum of *cCDI*[1] Comparisons	Sum of 0.5%	Sum of 99.5%	SIM-*cCDI*[1] Target
Pu-239	1.13E+04	1.03E+04	3.20E+03	3.76E+04	in range
U-238	4.96E+01	4.68E+01	8.40E+00	1.61E+02	in range
Cs-137	4.75E+04	1.81E+04	4.51E+03	2.31E+05	in range
Sr-90	1.68E+04	1.31E+04	3.74E+03	3.83E+04	in range

Note: [1]***Diediker (1999); cCDI: nomenclature for compare Cumulative Decayed Inventory (cCDI)***

The evaluation in this case is simple: Does the sum of the accepted set of literature values for the sites being compared fall within the 99% range? This is the test that is used to evaluate the model performance throughout the report at each level of comparison. In this case, the sum of the cCDI values for the analytes being evaluated falls within the computed uncertainty range,

and in fact, is relatively close to the estimated mean for three of four of the model values for these sites at this resolution, and all the results are well within the acceptance range. This performance gives some assurance that the model is providing useful output.

6.2.2 First-Order Comparison—SAC Selected Analytes by Closure Zone

For the purpose of first-order comparisons, the individual sites were grouped by SAC into 20 different categories (alternately called operable units or closure zones). These categories were determined by historical site use, geographic location, and facility association; although in some cases, there were no strong associations other than geographic. For the purpose of SIM, the unassigned 200 Area sites were subdivided into three separate worksheets to accommodate model architecture (using only one worksheet for that category as a single unit resulted in an output file that ran over the worksheet length).

The inventories for various analytes in the vadose zone are very highly skewed toward a select number of operable units. The 20 operable units/closure zones possess very different characteristics with respect to the inventories they contain. Table 6-4 illustrates the distribution of analyte by percentage of total inventory for those groupings for the analytes of interest to SAC, and Table 6-5 shows a qualitative comparison for the four specific analytes located in that group of sites being compared. Strong associations with plants/processes can be observed in this table, and there are few unexpected results.

Examples of specific dependencies can be observed in the PFP Zone for CCl_4 and Pu-239; PUREX Zone for tritium and I-129; NRDWL-BC Control Zone for Tc-99; and the S-U Farm Zone for Cs-137. The features of these wastes that influence the losses of these analytes are readily apparent (e.g., high concentrations of these analytes present in solution, inefficient or ineffective recovery operations, or entrained particulate); however, in other cases, there are subtleties present that require further interpretation in the development of these inputs. When these results are tied to the values in Table 6-2, risk and priority evaluations can be made.

Table 6-4. First Order Comparison—SAC Analytes of Interest by Operable Unit as a Percentage of Inventory (e.g., H-3, I-129, Tc-99, Cs-137, Sr-90, U-total, Pu-239, CCl_4, and Cr). (2 Sheets)

Location	Percent of Total Inventory								
	H-3	I-129	Tc-99	Cs-137	Sr-90	U-Total	Pu-239	CCl_4	Cr
200-E PONDS ZONE	30.70%	0.37%	0.31%	6.06%	0.66%	29.50%	0.42%	0.72%	0.69%
200-W PONDS ZONE	3.65%	4.77%	0.05%	0.43%	0.11%	2.60%	2.75%	4.07%	4.13%
B FARM ZONE	0.37%	4.46%	21.06%	8.09%	21.87%	5.83%	1.56%	0.00%	9.21%
B PLANT ZONE	1.32%	0.04%	0.64%	4.52%	0.44%	7.34%	0.34%	0.00%	2.22%
NRDWL-BC CONTROL ZONE	0.42%	13.68%	59.80%	2.25%	8.59%	1.81%	0.85%	0.00%	7.48%
PFP ZONE	0.00%	0.08%	0.00%	0.08%	0.32%	0.11%	86.15%	94.98%	1.14%
PUREX ZONE	45.79%	59.83%	0.34%	0.72%	2.26%	6.23%	2.80%	0.01%	3.79%
REDOX ZONE	6.85%	11.14%	0.83%	0.97%	5.10%	3.29%	1.39%	0.00%	11.05%
S-U FARM ZONE	0.13%	1.08%	5.18%	43.18%	3.31%	0.11%	0.03%	0.00%	0.39%
SEMIWORKS ZONE	0.05%	0.00%	0.00%	0.01%	0.21%	0.45%	0.00%	0.00%	18.40%
SOLID WASTE ZONE	0.07%	0.00%	0.00%	0.01%	0.05%	0.09%	0.07%	0.00%	0.21%

Table 6-4. First Order Comparison—SAC Analytes of Interest by Operable Unit as a Percentage of Inventory (e.g., H-3, I-129, Tc-99, Cs-137, Sr-90, U-total, Pu-239, CCl_4, and Cr). (2 Sheets)

Location	Percent of Total Inventory								
	H-3	I-129	Tc-99	Cs-137	Sr-90	U-Total	Pu-239	CCl_4	Cr
T FARM ZONE	2.99%	1.74%	7.41%	15.19%	16.95%	1.22%	3.46%	0.17%	20.25%
T PLANT ZONE	0.00%	1.08%	0.05%	0.31%	0.19%	0.07%	0.02%	0.00%	1.10%
U PLANT ZONE	6.92%	0.10%	1.56%	0.03%	0.06%	18.07%	0.00%	0.00%	0.73%
UNASSIGNED 200 AREA 1	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
UNASSIGNED 200 AREA 2	0.01%	0.58%	0.70%	0.84%	0.34%	0.01%	0.05%	0.01%	0.18%
UNASSIGNED 200 AREA	0.00%	0.00%	0.15%	1.86%	35.79%	0.00%	0.01%	0.00%	0.03%
UNASSIGNED 300 AREA	0.00%	0.80%	0.09%	0.62%	0.33%	22.95%	0.08%	0.00%	15.33%
WM ZONE	0.71%	0.01%	0.01%	0.00%	0.01%	0.29%	0.00%	0.04%	3.64%
WTP-ETF-A-C FARM ZONE	0.00%	0.24%	1.81%	14.83%	3.44%	0.00%	0.01%	0.00%	0.05%

The overall loss percentages of tritium and I-129 are elevated because of their volatility and solubility. They are also highly localized to certain disposal sites and geographic areas because of past waste disposal practices. These analytes were much more difficult for the contamination control measures in place at the separation plants to detect or contain.

That the vast majority of CCl_4 and Pu-239 was lost to the ground in the PFP Zone is logical; those discharges were essentially spent process effluent discharges of waste, and these analytes were principal components of those discharge streams.

Although the loss ratios for Sr-90 and Cs-137 are low, the inventories lost were disproportionately skewed to zones that had a large number of tank leaks and unplanned releases. Additionally, the presence of particulates in some of these losses affected the geographic distribution of cesium and strontium inventory.

In contrast to Cs-137, the case of Tc-99 is substantially different, even though it is considered completely soluble in the various waste stream environments, much as Cs-137 is. All three previously described loss characteristics are at work in this case. The relative decay rates of the two analytes are far different (Cs-137—30 years; Tc-99—213,000 years). Furthermore, although much more Tc-99 and Cs-137 were produced at later times in the Hanford Site's operating history, the impact of the change in waste management protocols had a disproportionate effect on Cs-137 (Cs-137 was routinely identified for reclamation and recycling, where Tc-99 rarely was; thus another factor in the observed difference); and the later Tc-99-bearing waste was principally discharged to the double-shell tanks, rather than to any liquid waste disposal sites. These factors dictate the substantial difference in loss observed between these radionuclides.

The losses for uranium are highly localized to areas that were used for disposing plant cold start waste, fuel rod production waste (300 Area), or uranium recycling byproduct waste. The distribution of chromium is somewhat different from the other analytes because it is present as a routine process chemical and also enters the system as a corrosion contaminant.

The following tables (Tables 6-5 to 6-9) provide the results of the comparison of the reference values to the 99% range computed by SIM. Again, in this case for purposes of comparison, if the reference value falls within the target interval, that is considered model agreement with observation; where there are significant discrepancies, those results require further investigation, review, and analysis. Table 6-5 provides a qualitative overview of the first order comparison results for each of the four analytes. At the first order level of comparison, SIM is finding at least three of the four analytes in question to be within the target interval.

Table 6-5. First Order Comparison—Qualitative Comparison for Four Analytes by Operable Unit

Operable Unit	Pu-239	U-238	Cs-137	Sr-90	1st Order Comparison
200-E Ponds Zone	in range	in range	in range	in range	100%
200-W Ponds Zone	in range	in range	in range	in range	100%
B Farm Zone	SIM high	in range	in range	in range	75%
B Plant Zone	SIM low	in range	in range	in range	75%
NRDWL-BC Control Zone	SIM high	in range	in range	in range	75%
PFP Zone	in range	in range	in range	in range	100%
PUREX Zone	in range	in range	in range	in range	100%
REDOX Zone	in range	in range	in range	in range	100%
Semiworks Zone	in range	in range	SIM high	in range	75%
Solid Waste Zone	in range	in range	SIM high	in range	75%
S-U Farm Zone	SIM low	in range	in range	in range	75%
T Farm Zone	in range	in range	in range	in range	100%
T Plant Zone	in range	in range	in range	in range	100%
U Plant Zone	SIM low	in range	in range	in range	75%
WM Zone	SIM low	in range	in range	in range	75%
WTP-ETF-A-C Farm Zone	in range	in range	in range	in range	100%
0th Order Comparison	in range	in range	in range	in range	100%

Tables 6-6 to 6-9 provide the individual results for each of the four specific SAC analytes of interest.

Table 6-6. Pu-239 Quantitative First Order Comparison by Operable Unit (Ci). (2 Sheets)

Operable Unit	Sum of Means	Sum of cCDI Values	Sum of 0.5%	Sum of 99.5%	SIM - cCDI Target
200-E Ponds Zone	5.03E+01	4.75E+01	2.38E+01	9.80E+01	in range
200-W Ponds Zone	3.12E+02	8.88E+01	6.55E+00	2.08E+03	in range
B Farm Zone	1.60E+02	7.55E+00	6.17E+01	2.81E+02	SIM high
B Plant Zone	4.43E-01	2.38E+01	5.24E-02	3.53E+00	SIM low
NRDWL-BC Control Zone	1.00E+02	1.65E+01	1.69E+01	2.66E+02	SIM high
PFP Zone	1.00E+04	9.77E+03	2.95E+03	3.26E+04	in range
PUREX Zone	3.36E+02	8.73E+01	5.36E+01	1.31E+03	in range

Table 6-6. Pu-239 Quantitative First Order Comparison by Operable Unit (Ci). (2 Sheets)

Operable Unit	Sum of Means	Sum of cCDI Values	Sum of 0.5%	Sum of 99.5%	SIM - cCDI Target
REDOX Zone	1.64E+02	1.16E+02	7.10E+01	2.99E+02	in range
Semiworks Zone	4.57E-01	7.79E-01	1.40E-02	2.21E+00	in range
Solid Waste Zone	8.09E+00	1.08E+01	3.37E+00	1.47E+01	in range
S-U Farm Zone	3.35E-03	1.42E-01	8.48E-04	8.48E-03	SIM low
T Farm Zone	1.34E+02	1.43E+02	1.50E+01	6.27E+02	in range
T Plant Zone	1.95E+00	9.42E-01	4.20E-02	1.78E+01	in range
U Plant Zone	1.41E-01	2.54E+01	3.00E-02	3.94E-01	SIM low
WM Zone	4.89E-02	2.28E-01	2.81E-02	8.22E-02	SIM low
WTP-ETF-A-C Farm Zone					No comparison
0th Order Comparison	1.13E+04	1.03E+04	3.20E+03	3.76E+04	in range

On inspection of the first order results for Pu-239, no particular trend is observed at the summary level. Two operable units are out of the target range on the high side, resulting from Tank Farms using contemporary solubility data as a basis in the HDW Model, where the historical data suggest a much lower value. Nine out of 16 operable units were within range, and the values are reasonably close: four are out of range on the low side and one does not have a comparison. The acceptance interval range for this analyte varies as a function of operable unit, but the observed spans are approximately one to one and a half orders of magnitude.

Table 6-7. U-238 Quantitative First Comparison by Operable Unit (Ci)

Operable Unit	Sum of Mean	Sum of cCDI Compare	Sum of 0.5%	Sum of 99.5%	SIM - cCDI Target
200-E Ponds Zone	2.06E+01	2.01E+01	1.78E+00	8.13E+01	in range
200-W Ponds Zone	1.76E+00	2.28E+00	5.45E-01	3.90E+00	in range
B Farm Zone	5.85E-01	4.68E-01	1.12E-01	1.39E+00	in range
B Plant Zone	5.05E+00	7.23E+00	9.06E-01	1.31E+01	in range
NRDWL-BC Control Zone	1.25E+00	1.80E+00	1.22E-01	4.04E+00	in range
PFP Zone	7.11E-02	2.85E-02	2.56E-03	7.64E-01	in range
PUREX Zone	4.23E+00	1.46E+00	7.43E-01	1.67E+01	in range
REDOX Zone	2.25E+00	1.74E+00	8.39E-01	4.34E+00	in range
Semiworks Zone	3.16E-01	1.33E-01	8.94E-02	6.86E-01	in range
Solid Waste Zone	6.41E-02	1.65E-01	2.84E-03	4.18E-01	in range
S-U Farm Zone	6.56E-03	6.32E-03	2.08E-04	1.78E-02	in range
T Farm Zone	7.09E-01	2.69E-01	4.41E-02	3.30E+00	in range
T Plant Zone	3.96E-02	7.12E-03	6.16E-04	2.88E-01	in range
U Plant Zone	1.24E+01	1.08E+01	3.20E+00	3.02E+01	in range
WM Zone	2.00E-01	2.32E-01	1.49E-02	6.09E-01	in range
WTP-ETF-A-C Farm Zone					No comparison
0th Order Comparison	4.96E+01	4.68E+01	8.40E+00	1.61E+02	in range

Evaluating the first order results for U-238 reveals no discernable trend—15 out of 16 operable units were within range with most of the values quite close between the SIM result and cCDI; one operable unit does not have a comparison.

Table 6-8. Cs-137 Quantitative First Comparison by Operable Unit

Operable Unit	Sum of Mean	Sum of cCDI Compare	Sum of 0.5%	Sum of 99.5%	SIM - cCDI Target
200-E Ponds Zone	1.36E+04	8.46E+02	6.02E+02	6.39E+04	in range
200-W Ponds Zone	9.45E+02	2.11E+02	1.16E+02	4.00E+03	in range
B Farm Zone	8.16E+03	3.73E+03	9.42E+02	1.84E+04	in range
B Plant Zone	9.60E+03	6.73E+02	7.67E+01	1.09E+05	in range
NRDWL-BC Control Zone	4.96E+03	3.32E+03	9.50E+02	1.11E+04	in range
PFP Zone	1.63E+02	1.63E+02	8.08E+01	2.55E+02	in range
PUREX Zone	1.47E+03	1.33E+03	1.03E+02	5.43E+03	in range
REDOX Zone	2.10E+03	1.67E+03	1.01E+03	3.60E+03	in range
Semiworks Zone	1.85E+01	8.24E-01	3.92E+00	4.04E+01	SIM high
Solid Waste Zone	1.25E+01	3.60E+00	5.26E+00	2.22E+01	SIM high
S-U Farm Zone	4.22E+01	1.74E+01	3.53E+00	1.46E+02	in range
T Farm Zone	6.15E+03	6.04E+03	6.10E+02	1.44E+04	in range
T Plant Zone	2.04E+02	1.40E+01	3.09E+00	7.25E+02	in range
U Plant Zone	7.10E+01	1.24E+01	1.15E+00	4.02E+02	in range
WM Zone	5.51E+00	4.83E+00	2.70E+00	9.06E+00	in range
WTP-ETF-A-C Farm Zone	1.45E+01	1.11E+01	3.04E-03	7.93E+01	in range
0th Order Comparison	4.75E+04	1.81E+04	4.51E+03	2.31E+05	in range

On inspection of the first order results for Cs-137, a trend is definitely observed—14 out of 16 operable units are in range, but approximately half of the model results are substantially higher than the reference values and two of the operable unit values are outside the reference interval on the high side, suggesting that the current model convention for Cs-137 solubility may be too high. When individual operable unit comparisons between the model values and reference values are made, eight model results are distinctly higher in value. In this case, distinctly higher or lower than the reference value means within a factor of three. The span of the acceptance interval for this analyte is consistently large, ranging over two and a half orders of magnitude in some cases.

Table 6-9. Sr-90 Quantitative First Order Comparison by Operable Unit.

Operable Unit	Sum of Median	Sum of cCDI compare	Sum of 0.5%	Sum of 99.5%	SIM - cCDI target
200-E Ponds Zone	3.41E+02	3.31E+02	9.52E+01	1.15E+03	in range
200-W Ponds Zone	5.56E+01	2.64E+02	5.23E+00	3.62E+02	in range
B Farm Zone	6.10E+03	5.54E+03	8.20E+02	1.29E+04	in range
B Plant Zone	2.00E+02	1.25E+02	3.41E+01	9.85E+02	in range
NRDWL-BC Control Zone	4.43E+03	2.51E+03	9.69E+02	9.59E+03	in range
PFP Zone	1.58E+02	1.58E+02	8.45E+01	2.46E+02	in range
PUREX Zone	1.19E+03	1.25E+03	8.68E+01	4.30E+03	in range
REDOX Zone	2.62E+03	2.12E+03	1.43E+03	4.30E+03	in range
Semiworks Zone	1.08E+02	1.35E+02	1.47E+01	2.89E+02	in range
Solid Waste Zone	1.14E+01	6.14E+00	3.99E+00	2.05E+01	in range
S-U Farm Zone	5.07E-01	4.51E-01	5.55E-02	1.49E+00	in range
T Farm Zone	1.54E+03	5.89E+02	1.95E+02	3.97E+03	in range
T Plant Zone	3.65E+01	1.29E+01	2.19E+00	1.31E+02	in range
U Plant Zone	3.07E+01	1.03E+01	1.18E+00	1.22E+02	in range
WM Zone	2.89E+00	2.59E+00	1.35E+00	5.38E+00	in range
WTP-ETF-A-C Farm Zone					No comparison
0th Order Comparison	1.68E+04	1.31E+04	3.74E+03	3.83E+04	in range

Reviewing the first order results for Sr-90 reveals no strong trend. Indeed, all of the observed results are within the acceptance interval, with one no comparison, and most of the model results are close to the reference values (with differences of less than 50%). There is a modestly positive trend for this analyte; six operable unit results are distinctly higher; and one is distinctly lower than the reference value, where the differences are greater than 50%.

The following first order comparisons are for the SAC analytes of interest by site as a percentage of inventory (e.g., H-3, I-129, Tc-99, Cs-137, Sr-90, U-total, Pu-239, CCl_4, and Cr). Both absolute inventory quantities and relative distributions are provided in Tables 6-10 to 6-18.

Table 6-10. Distribution of H-3 by Category with Respect to the Total Inventory

Operable Unit	Resolution	Analyte	Inv. Unit	Amt.	% of Total Inv.
200-E PONDS ZONE	Summation	H-3	Ci	5.44E+04	30.70%
200-W PONDS ZONE	Summation	H-3	Ci	6.46E+03	3.65%
B FARM ZONE	Summation	H-3	Ci	6.51E+02	0.37%
B PLANT ZONE	Summation	H-3	Ci	2.34E+03	1.32%
NRDWL-BC CONTROL ZONE	Summation	H-3	Ci	7.42E+02	0.42%
PFP ZONE	Summation	H-3	Ci	1.55E-03	0.00%
PUREX ZONE	Summation	H-3	Ci	8.11E+04	45.79%
REDOX ZONE	Summation	H-3	Ci	1.21E+04	6.85%
S-U FARM ZONE	Summation	H-3	Ci	2.32E+02	0.13%
SEMIWORKS ZONE	Summation	H-3	Ci	9.17E+01	0.05%
SOLID WASTE ZONE	Summation	H-3	Ci	1.30E+02	0.07%
T FARM ZONE	Summation	H-3	Ci	5.30E+03	2.99%
T PLANT ZONE	Summation	H-3	Ci	1.45E+00	0.00%
U PLANT ZONE	Summation	H-3	Ci	1.23E+04	6.92%
UNASSIGNED 200 AREA 1	Summation	H-3	Ci	1.25E-05	0.00%
UNASSIGNED 200 AREA 2	Summation	H-3	Ci	2.49E+01	0.01%
UNASSIGNED 200 AREA	Summation	H-3	Ci	6.19E-02	0.00%
UNASSIGNED 300 AREA	Summation	H-3	Ci	1.52E+00	0.00%
WM ZONE	Summation	H-3	Ci	1.25E+03	0.71%
WTP-ETF-A-C FARM ZONE	Summation	H-3	Ci	3.69E+00	0.00%
Total	Summation	H-3	Ci	1.77E+05	

Table 6-11. Distribution of Tc-99 by Category with Respect to the Total Inventory

Operable Unit	Resolution	Analyte	Inv. Unit	Amt.	% of Total Inv.
200-E PONDS ZONE	Summation	Tc-99	Ci	2.15E+00	0.31%
200-W PONDS ZONE	Summation	Tc-99	Ci	3.45E-01	0.05%
B FARM ZONE	Summation	Tc-99	Ci	1.45E+02	21.06%
B PLANT ZONE	Summation	Tc-99	Ci	4.41E+00	0.64%
NRDWL-BC CONTROL ZONE	Summation	Tc-99	Ci	4.11E+02	59.80%
PFP ZONE	Summation	Tc-99	Ci	3.81E-03	0.00%
PUREX ZONE	Summation	Tc-99	Ci	2.30E+00	0.34%
REDOX ZONE	Summation	Tc-99	Ci	5.68E+00	0.83%
S-U FARM ZONE	Summation	Tc-99	Ci	3.56E+01	5.18%
SEMIWORKS ZONE	Summation	Tc-99	Ci	9.19E-03	0.00%
SOLID WASTE ZONE	Summation	Tc-99	Ci	2.32E-02	0.00%
T FARM ZONE	Summation	Tc-99	Ci	5.09E+01	7.41%
T PLANT ZONE	Summation	Tc-99	Ci	3.11E-01	0.05%
U PLANT ZONE	Summation	Tc-99	Ci	1.07E+01	1.56%
UNASSIGNED 200 AREA 1	Summation	Tc-99	Ci	7.18E-06	0.00%
UNASSIGNED 200 AREA 2	Summation	Tc-99	Ci	4.84E+00	0.70%
UNASSIGNED 200 AREA	Summation	Tc-99	Ci	1.03E+00	0.15%
UNASSIGNED 300 AREA	Summation	Tc-99	Ci	6.28E-01	0.09%
WM ZONE	Summation	Tc-99	Ci	6.68E-02	0.01%
WTP-ETF-A-C FARM ZONE	Summation	Tc-99	Ci	1.25E+01	1.81%
Total	Summation	Tc-99	Ci	6.87E+02	

Table 6-12. Distribution of I-129 by Category with Respect to the Total Inventory

Operable Unit	Resolution	Analyte	Inv. Unit	Amt.	% of Total Inv.
200-E PONDS ZONE	Summation	I-129	Ci	1.73E-02	0.37%
200-W PONDS ZONE	Summation	I-129	Ci	2.25E-01	4.77%
B FARM ZONE	Summation	I-129	Ci	2.10E-01	4.46%
B PLANT ZONE	Summation	I-129	Ci	1.69E-03	0.04%
NRDWL-BC CONTROL ZONE	Summation	I-129	Ci	6.45E-01	13.68%
PFP ZONE	Summation	I-129	Ci	3.71E-03	0.08%
PUREX ZONE	Summation	I-129	Ci	2.82E+00	59.83%
REDOX ZONE	Summation	I-129	Ci	5.25E-01	11.14%
S-U FARM ZONE	Summation	I-129	Ci	5.10E-02	1.08%
SEMIWORKS ZONE	Summation	I-129	Ci	8.58E-06	0.00%
SOLID WASTE ZONE	Summation	I-129	Ci	1.43E-06	0.00%
T FARM ZONE	Summation	I-129	Ci	8.22E-02	1.74%
T PLANT ZONE	Summation	I-129	Ci	5.11E-02	1.08%
U PLANT ZONE	Summation	I-129	Ci	4.93E-03	0.10%
UNASSIGNED 200 AREA 1	Summation	I-129	Ci	1.06E-07	0.00%
UNASSIGNED 200 AREA 2	Summation	I-129	Ci	2.73E-02	0.58%
UNASSIGNED 200 AREA	Summation	I-129	Ci	6.74E-05	0.00%
UNASSIGNED 300 AREA	Summation	I-129	Ci	3.75E-02	0.80%
WM ZONE	Summation	I-129	Ci	4.36E-04	0.01%
WTP-ETF-A-C FARM ZONE	Summation	I-129	Ci	1.12E-02	0.24%
Total	Summation	I-129	Ci	4.72E+00	

Table 6-13. Distribution of Cs-137 by Category with Respect to the Total Inventory

Operable Unit	Resolution	Analyte	Inv. Unit	Amt.	% of Total Inv.
200-E PONDS ZONE	Summation	Cs-137	Ci	1.35E+04	6.06%
200-W PONDS ZONE	Summation	Cs-137	Ci	9.65E+02	0.43%
B FARM ZONE	Summation	Cs-137	Ci	1.80E+04	8.09%
B PLANT ZONE	Summation	Cs-137	Ci	1.01E+04	4.52%
NRDWL-BC CONTROL ZONE	Summation	Cs-137	Ci	5.00E+03	2.25%
PFP ZONE	Summation	Cs-137	Ci	1.70E+02	0.08%
PUREX ZONE	Summation	Cs-137	Ci	1.60E+03	0.72%
REDOX ZONE	Summation	Cs-137	Ci	2.16E+03	0.97%
S-U FARM ZONE	Summation	Cs-137	Ci	9.61E+04	43.18%
SEMIWORKS ZONE	Summation	Cs-137	Ci	1.82E+01	0.01%
SOLID WASTE ZONE	Summation	Cs-137	Ci	1.59E+01	0.01%
T FARM ZONE	Summation	Cs-137	Ci	3.38E+04	15.19%
T PLANT ZONE	Summation	Cs-137	Ci	6.81E+02	0.31%
U PLANT ZONE	Summation	Cs-137	Ci	7.19E+01	0.03%
UNASSIGNED 200 AREA 1	Summation	Cs-137	Ci	1.97E-02	0.00%
UNASSIGNED 200 AREA 2	Summation	Cs-137	Ci	1.87E+03	0.84%
UNASSIGNED 200 AREA	Summation	Cs-137	Ci	4.15E+03	1.86%
UNASSIGNED 300 AREA	Summation	Cs-137	Ci	1.39E+03	0.62%
WM ZONE	Summation	Cs-137	Ci	5.50E+00	0.00%
WTP-ETF-A-C FARM ZONE	Summation	Cs-137	Ci	3.30E+04	14.83%
Total	Summation	Cs-137	Ci	2.23E+05	

Table 6-14. Distribution of Sr-90 by Category with Respect to the Total Inventory

Operable Unit	Resolution	Analyte	Inv. Unit	Amt.	% of Total Inv.
200-E PONDS ZONE	Summation	Sr-90	Ci	3.38E+02	0.66%
200-W PONDS ZONE	Summation	Sr-90	Ci	5.52E+01	0.11%
B FARM ZONE	Summation	Sr-90	Ci	1.13E+04	21.87%
B PLANT ZONE	Summation	Sr-90	Ci	2.25E+02	0.44%
NRDWL-BC CONTROL ZONE	Summation	Sr-90	Ci	4.43E+03	8.59%
PFP ZONE	Summation	Sr-90	Ci	1.65E+02	0.32%
PUREX ZONE	Summation	Sr-90	Ci	1.16E+03	2.26%
REDOX ZONE	Summation	Sr-90	Ci	2.63E+03	5.10%
S-U FARM ZONE	Summation	Sr-90	Ci	1.70E+03	3.31%
SEMIWORKS ZONE	Summation	Sr-90	Ci	1.08E+02	0.21%
SOLID WASTE ZONE	Summation	Sr-90	Ci	2.64E+01	0.05%
T FARM ZONE	Summation	Sr-90	Ci	8.74E+03	16.95%
T PLANT ZONE	Summation	Sr-90	Ci	9.69E+01	0.19%
U PLANT ZONE	Summation	Sr-90	Ci	3.12E+01	0.06%
UNASSIGNED 200 AREA 1	Summation	Sr-90	Ci	9.06E-04	0.00%
UNASSIGNED 200 AREA 2	Summation	Sr-90	Ci	1.74E+02	0.34%
UNASSIGNED 200 AREA	Summation	Sr-90	Ci	1.84E+04	35.79%
UNASSIGNED 300 AREA	Summation	Sr-90	Ci	1.69E+02	0.33%
WM ZONE	Summation	Sr-90	Ci	2.87E+00	0.01%
WTP-ETF-A-C FARM ZONE	Summation	Sr-90	Ci	1.77E+03	3.44%
Total	Summation	Sr-90	Ci	5.15E+04	

Table 6-15. Distribution of U-Total by Category with Respect to the Total Inventory

Operable Unit	Resolution	Analyte	Inv. Unit	Amt.	% of Total Inv.
200-E PONDS ZONE	Summation	U-Total	kg	6.08E+04	29.50%
200-W PONDS ZONE	Summation	U-Total	kg	5.37E+03	2.60%
B FARM ZONE	Summation	U-Total	kg	1.20E+04	5.83%
B PLANT ZONE	Summation	U-Total	kg	1.51E+04	7.34%
NRDWL-BC CONTROL ZONE	Summation	U-Total	kg	3.74E+03	1.81%
PFP ZONE	Summation	U-Total	kg	2.23E+02	0.11%
PUREX ZONE	Summation	U-Total	kg	1.28E+04	6.23%
REDOX ZONE	Summation	U-Total	kg	6.79E+03	3.29%
S-U FARM ZONE	Summation	U-Total	kg	2.19E+02	0.11%
SEMIWORKS ZONE	Summation	U-Total	kg	9.35E+02	0.45%
SOLID WASTE ZONE	Summation	U-Total	kg	1.91E+02	0.09%
T FARM ZONE	Summation	U-Total	kg	2.50E+03	1.22%
T PLANT ZONE	Summation	U-Total	kg	1.41E+02	0.07%
U PLANT ZONE	Summation	U-Total	kg	3.72E+04	18.07%
UNASSIGNED 200 AREA 1	Summation	U-Total	kg	8.48E-02	0.00%
UNASSIGNED 200 AREA 2	Summation	U-Total	kg	3.01E+01	0.01%
UNASSIGNED 200 AREA	Summation	U-Total	kg	5.96E+00	0.00%
UNASSIGNED 300 AREA	Summation	U-Total	kg	4.73E+04	22.95%
WM ZONE	Summation	U-Total	kg	6.07E+02	0.29%
WTP-ETF-A-C FARM ZONE	Summation	U-Total	kg	4.75E+00	0.00%
Total	Summation	U-Total	kg	2.06E+05	

Table 6-16. Distribution of Pu-239 by Category with Respect to the Total Inventory

Operable Unit	Resolution	Analyte	Inv. Unit	Amt.	% of Total Inv.
200-E PONDS ZONE	Summation	Pu-239	Ci	5.00E+01	0.42%
200-W PONDS ZONE	Summation	Pu-239	Ci	3.24E+02	2.75%
B FARM ZONE	Summation	Pu-239	Ci	1.83E+02	1.56%
B PLANT ZONE	Summation	Pu-239	Ci	4.03E+01	0.34%
NRDWL-BC CONTROL ZONE	Summation	Pu-239	Ci	1.00E+02	0.85%
PFP ZONE	Summation	Pu-239	Ci	1.02E+04	86.15%
PUREX ZONE	Summation	Pu-239	Ci	3.30E+02	2.80%
REDOX ZONE	Summation	Pu-239	Ci	1.64E+02	1.39%
S-U FARM ZONE	Summation	Pu-239	Ci	4.06E+00	0.03%
SEMIWORKS ZONE	Summation	Pu-239	Ci	4.71E-01	0.00%
SOLID WASTE ZONE	Summation	Pu-239	Ci	8.10E+00	0.07%
T FARM ZONE	Summation	Pu-239	Ci	4.08E+02	3.46%
T PLANT ZONE	Summation	Pu-239	Ci	2.06E+00	0.02%
U PLANT ZONE	Summation	Pu-239	Ci	1.43E-01	0.00%
UNASSIGNED 200 AREA 1	Summation	Pu-239	Ci	1.86E-04	0.00%
UNASSIGNED 200 AREA 2	Summation	Pu-239	Ci	5.46E+00	0.05%
UNASSIGNED 200 AREA	Summation	Pu-239	Ci	1.13E+00	0.01%
UNASSIGNED 300 AREA	Summation	Pu-239	Ci	9.96E+00	0.08%
WM ZONE	Summation	Pu-239	Ci	4.87E-02	0.00%
WTP-ETF-A-C FARM ZONE	Summation	Pu-239	Ci	7.61E-01	0.01%
Total	Summation	Pu-239	Ci	1.18E+04	

Table 6-17. Distribution of CCl_4 by Category with Respect to the Total Inventory

Operable Unit	Resolution	Analyte	Inv. Unit	Amt.	% of Total Inv.
200-E PONDS ZONE	Summation	CCl_4	kg	6.88E+03	0.72%
200-W PONDS ZONE	Summation	CCl_4	kg	3.91E+04	4.07%
B FARM ZONE	Summation	CCl_4	kg	0.00E+00	0.00%
B PLANT ZONE	Summation	CCl_4	kg	0.00E+00	0.00%
NRDWL-BC CONTROL ZONE	Summation	CCl_4	kg	0.00E+00	0.00%
PFP ZONE	Summation	CCl_4	kg	9.12E+05	94.98%
PUREX ZONE	Summation	CCl_4	kg	6.68E+01	0.01%
REDOX ZONE	Summation	CCl_4	kg	0.00E+00	0.00%
S-U FARM ZONE	Summation	CCl_4	kg	0.00E+00	0.00%
SEMIWORKS ZONE	Summation	CCl_4	kg	0.00E+00	0.00%
SOLID WASTE ZONE	Summation	CCl_4	kg	0.00E+00	0.00%
T FARM ZONE	Summation	CCl_4	kg	1.66E+03	0.17%
T PLANT ZONE	Summation	CCl_4	kg	0.00E+00	0.00%
U PLANT ZONE	Summation	CCl_4	kg	0.00E+00	0.00%
UNASSIGNED 200 AREA 1	Summation	CCl_4	kg	0.00E+00	0.00%
UNASSIGNED 200 AREA 2	Summation	CCl_4	kg	1.29E+02	0.01%
UNASSIGNED 200 AREA	Summation	CCl_4	kg	0.00E+00	0.00%
UNASSIGNED 300 AREA	Summation	CCl_4	kg	0.00E+00	0.00%
WM ZONE	Summation	CCl_4	kg	3.62E+02	0.04%
WTP-ETF-A-C FARM ZONE	Summation	CCl_4	kg	0.00E+00	0.00%
Total	Summation	CCl_4	kg	9.60E+05	

Table 6-18. Distribution of Cr by Category with Respect to the Total Inventory

Operable Unit	Resolution	Analyte	Inv. Unit	Amt.	% of Total Inv.
200-E PONDS ZONE	Summation	Cr	kg	2.17E+03	0.69%
200-W PONDS ZONE	Summation	Cr	kg	1.30E+04	4.13%
B FARM ZONE	Summation	Cr	kg	2.89E+04	9.21%
B PLANT ZONE	Summation	Cr	kg	6.96E+03	2.22%
NRDWL-BC CONTROL ZONE	Summation	Cr	kg	2.35E+04	7.48%
PFP ZONE	Summation	Cr	kg	3.57E+03	1.14%
PUREX ZONE	Summation	Cr	kg	1.19E+04	3.79%
REDOX ZONE	Summation	Cr	kg	3.47E+04	11.05%
S-U FARM ZONE	Summation	Cr	kg	1.22E+03	0.39%
SEMIWORKS ZONE	Summation	Cr	kg	5.77E+04	18.40%
SOLID WASTE ZONE	Summation	Cr	kg	6.54E+02	0.21%
T FARM ZONE	Summation	Cr	kg	6.35E+04	20.25%
T PLANT ZONE	Summation	Cr	kg	3.46E+03	1.10%
U PLANT ZONE	Summation	Cr	kg	2.29E+03	0.73%
UNASSIGNED 200 AREA 1	Summation	Cr	kg	4.92E-02	0.00%
UNASSIGNED 200 AREA 2	Summation	Cr	kg	5.64E+02	0.18%
UNASSIGNED 200 AREA	Summation	Cr	kg	7.90E+01	0.03%
UNASSIGNED 300 AREA	Summation	Cr	kg	4.81E+04	15.33%
WM ZONE	Summation	Cr	kg	1.14E+04	3.64%
WTP-ETF-A-C FARM ZONE	Summation	Cr	kg	1.42E+02	0.05%
Total	Summation	Cr	kg	3.14E+05	

Table 6-19 provides a summary of the mean values lost to the environment as a function of time for the SAC analytes of interest. Figures 6-11 to 6-19 illustrate these trends graphically.

Table 6-19. Annual Mean Values Lost to Environment (Radionuclides Decayed to 1/1/2001). (2 Sheets)

Year	H-3 (Ci)	Sr-90 (Ci)	Tc-99 (Ci)	I-129 (Ci)	Cs-137 (Ci)	U Total (kg)	Pu-239 (Ci)	CCl_4 (kg)	Cr (kg)
1944	1.17E-01	1.30E+01	4.83E-02	6.25E-04	1.07E+02	1.35E+03	6.07E-02	0.00E+00	1.51E+03
1945	1.52E-01	2.63E+01	6.48E-02	3.50E-03	1.49E+02	1.35E+03	2.82E+01	1.59E+01	5.56E+03
1946	2.18E-01	3.49E+01	7.41E-02	3.51E-03	1.64E+02	1.37E+03	7.29E+01	4.91E+00	7.14E+03
1947	3.01E-01	9.67E+01	1.63E-01	3.55E-03	3.69E+02	1.40E+03	1.06E+02	6.12E+01	6.68E+03
1948	1.59E-01	1.07E+02	1.00E-01	3.52E-03	2.43E+02	1.44E+03	1.48E+02	6.54E+01	8.94E+03
1949	1.59E-01	1.11E+02	1.03E-01	3.42E-03	2.48E+02	1.45E+03	1.60E+02	4.26E+03	9.07E+03
1950	2.51E-01	1.68E+02	1.52E-01	4.20E-03	3.62E+02	1.49E+03	1.74E+02	8.53E+03	1.06E+04
1951	5.34E+00	2.51E+03	2.60E+00	5.20E-03	4.98E+03	1.17E+04	1.48E+02	8.53E+03	2.49E+04
1952	6.44E+02	1.46E+02	2.26E+00	1.11E-02	3.49E+02	6.29E+03	9.01E+01	5.48E+03	2.39E+04
1953	2.61E+03	5.02E+02	5.56E+00	5.40E-02	1.32E+03	1.08E+04	6.08E+01	1.78E+03	3.12E+04
1954	2.61E+03	3.15E+03	3.40E+01	1.57E-01	1.22E+04	1.59E+04	9.30E+01	1.81E+03	3.78E+04
1955	2.82E+03	4.95E+03	1.13E+02	2.17E-01	3.06E+03	6.00E+04	2.06E+02	7.69E+03	3.59E+04
1956	7.71E+03	3.55E+03	2.31E+02	5.50E-01	8.36E+03	1.83E+04	3.83E+02	3.41E+04	1.66E+04
1957	3.85E+03	2.12E+04	1.68E+02	4.29E-01	8.09E+03	6.89E+03	3.67E+02	3.48E+04	1.31E+04
1958	5.70E+03	4.56E+02	2.22E+01	2.78E-01	4.61E+03	5.56E+03	3.20E+02	3.42E+04	4.49E+03
1959	6.05E+03	3.40E+02	1.00E+00	2.50E-01	2.24E+03	3.00E+03	3.79E+02	4.26E+04	2.21E+03

Table 6-19. Annual Mean Values Lost to Environment (Radionuclides Decayed to 1/1/2001). (2 Sheets)

Year	H-3 (Ci)	Sr-90 (Ci)	Tc-99 (Ci)	I-129 (Ci)	Cs-137 (Ci)	U Total (kg)	Pu-239 (Ci)	CCl_4 (kg)	Cr (kg)
1960	5.70E+03	1.03E+02	2.84E-01	2.91E-01	6.56E+01	3.92E+03	5.89E+02	6.86E+04	3.02E+03
1961	3.87E+03	1.03E+02	2.37E-01	1.88E-01	7.22E+01	3.35E+03	4.72E+02	6.42E+04	3.70E+03
1962	5.31E+03	1.16E+02	2.53E-01	2.68E-01	8.26E+01	3.40E+03	2.44E+02	3.23E+04	3.45E+03
1963	6.30E+03	2.81E+02	6.28E+00	2.34E-01	1.80E+04	3.66E+03	1.66E+02	9.34E+03	4.35E+03
1964	8.38E+03	3.26E+02	2.22E+00	2.70E-01	7.52E+03	3.92E+03	6.25E+02	2.13E+04	3.16E+03
1965	8.96E+03	1.44E+03	5.98E+00	2.76E-01	1.90E+04	3.68E+03	6.32E+02	2.15E+04	6.38E+03
1966	7.21E+03	8.71E+02	1.54E+01	2.29E-01	4.80E+04	5.54E+03	9.52E+02	3.90E+04	1.31E+04
1967	1.74E+04	1.77E+03	8.45E-01	1.98E-01	2.14E+03	3.12E+03	9.75E+02	6.75E+04	4.45E+03
1968	1.56E+04	9.52E+02	3.47E+00	1.64E-01	1.74E+03	2.61E+03	1.79E+03	1.98E+05	3.67E+03
1969	1.03E+04	1.76E+02	1.51E+00	1.02E-01	3.30E+03	2.27E+03	7.06E+02	6.53E+04	3.57E+03
1970	5.63E+03	2.63E+01	7.35E-02	3.56E-02	5.11E+01	2.24E+03	4.61E+02	4.20E+04	3.26E+03
1971	7.34E+03	2.32E+02	6.67E+00	5.08E-02	2.34E+04	2.59E+03	5.94E+02	4.95E+04	2.96E+03
1972	5.14E+03	1.10E+03	3.44E+00	2.57E-02	2.81E+03	2.29E+03	5.85E+02	6.17E+04	2.94E+03
1973	2.69E+03	6.20E+03	4.15E+01	3.27E-02	2.29E+04	1.64E+03	1.74E+02	1.89E+04	3.13E+03
1974	3.36E+03	4.36E+01	1.23E+00	6.24E-03	1.37E+03	1.64E+03	8.56E-01	7.44E+02	2.30E+03
1975	1.57E+03	5.58E+01	1.74E+00	5.58E-03	3.78E+03	1.79E+03	1.15E+00	4.75E+02	2.11E+03
1976	6.19E+02	2.01E+01	3.55E-01	2.99E-03	6.18E+02	4.72E+02	1.80E+00	1.62E+02	7.34E+02
1977	4.87E+02	7.47E+01	4.39E+00	9.09E-03	8.07E+03	6.50E+02	2.31E+00	1.62E+01	6.98E+02
1978	2.86E+02	3.06E-01	1.60E-02	4.30E-03	1.30E+01	5.01E+02	1.83E+00	1.62E+01	5.57E+02
1979	4.01E+02	2.53E-01	1.02E-02	6.83E-03	5.77E+00	7.02E+02	2.30E+00	1.62E+01	5.90E+02
1980	4.85E+02	2.68E-01	8.43E-03	1.16E-02	4.52E+00	7.07E+02	5.13E+00	8.08E+02	5.83E+02
1981	5.10E+01	2.18E-01	7.42E-03	1.95E-02	1.10E+00	5.35E+02	4.80E+00	8.08E+02	5.50E+02
1982	7.04E+02	2.67E+01	1.42E+00	1.84E-02	1.51E+02	5.82E+02	5.16E+00	8.08E+02	4.91E+02
1983	1.18E+03	9.94E+00	2.06E-02	4.04E-02	1.14E+01	9.18E+02	6.67E+00	1.31E+03	4.86E+02
1984	5.98E+03	4.35E+01	6.31E-02	7.19E-02	5.02E+01	1.37E+03	6.57E+00	1.67E+03	4.54E+02
1985	5.87E+03	6.80E+01	6.24E-02	7.04E-02	7.60E+01	1.09E+03	6.96E+00	1.82E+03	4.62E+02
1986	3.23E+03	5.16E+01	5.06E-02	5.06E-02	5.85E+01	7.83E+02	6.26E+00	1.88E+03	4.37E+02
1987	2.65E+03	7.91E+01	5.13E+00	2.62E-02	6.56E+03	4.60E+02	5.78E+00	2.32E+03	4.92E+02
1988	2.75E+03	6.10E+01	4.52E+00	2.08E-02	5.94E+03	5.36E+02	5.78E+00	2.52E+03	4.66E+02
1989	1.07E+03	1.23E+00	5.07E-03	7.34E-03	1.71E+00	4.32E+02	6.43E+00	1.32E+03	4.07E+02
1990	5.50E+02	2.98E-01	3.73E-03	2.04E-03	1.79E+00	2.02E+02	2.47E+00	0.00E+00	4.13E+02
1991	5.29E+02	1.59E-01	4.21E-03	5.47E-04	2.55E+00	2.25E+02	2.47E+00	0.00E+00	3.52E+02
1992	5.15E+02	1.91E-01	3.63E-03	1.39E-03	2.04E+00	4.56E+00	3.82E-01	4.82E+01	8.72E+01
1993	6.72E+02	4.54E-01	4.01E-03	1.34E-03	1.94E+00	6.56E+00	5.89E-01	0.00E+00	8.18E+01
1994	5.94E+02	1.19E+00	3.77E-03	1.42E-05	1.21E+00	1.45E+00	9.65E-01	0.00E+00	1.34E+02
1995	5.71E+02	4.31E-01	3.24E-03	1.36E-05	3.64E-01	5.70E-01	5.93E-01	0.00E+00	7.04E+01
1996	7.11E+02	1.11E+00	2.27E-03	1.35E-06	2.52E-01	1.17E+00	1.06E+00	0.00E+00	1.04E+00
1997	3.87E+02	3.54E-01	1.74E-05	1.29E-08	2.54E-03	3.73E-01	4.44E-01	0.00E+00	7.17E-01
1998	1.06E-07	2.12E-06	7.32E-08	1.28E-10	2.66E-04	8.01E-04	2.38E-08	0.00E+00	5.06E-01
1999	1.04E-07	2.12E-06	6.36E-08	1.22E-10	2.64E-04	6.81E-05	9.97E-09	0.00E+00	4.39E-02
2000	1.11E-07	2.27E-06	6.85E-08	2.34E-06	2.84E-04	4.11E-04	1.69E-08	0.00E+00	1.93E+00
2001	1.04E-07	2.12E-06	6.39E-08	1.22E-10	2.64E-04	4.00E-04	1.61E-08	0.00E+00	2.53E-01

Figure 6-11. Annual Tritium Losses

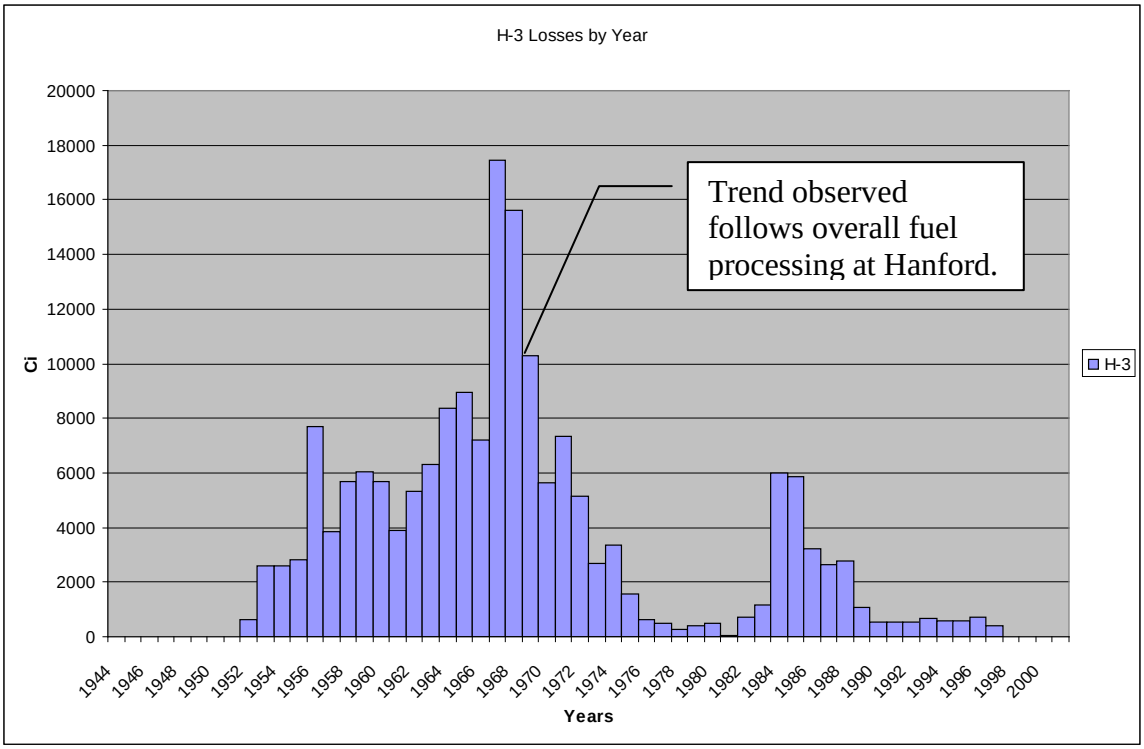


Figure 6-12. Annual Sr-90 Losses

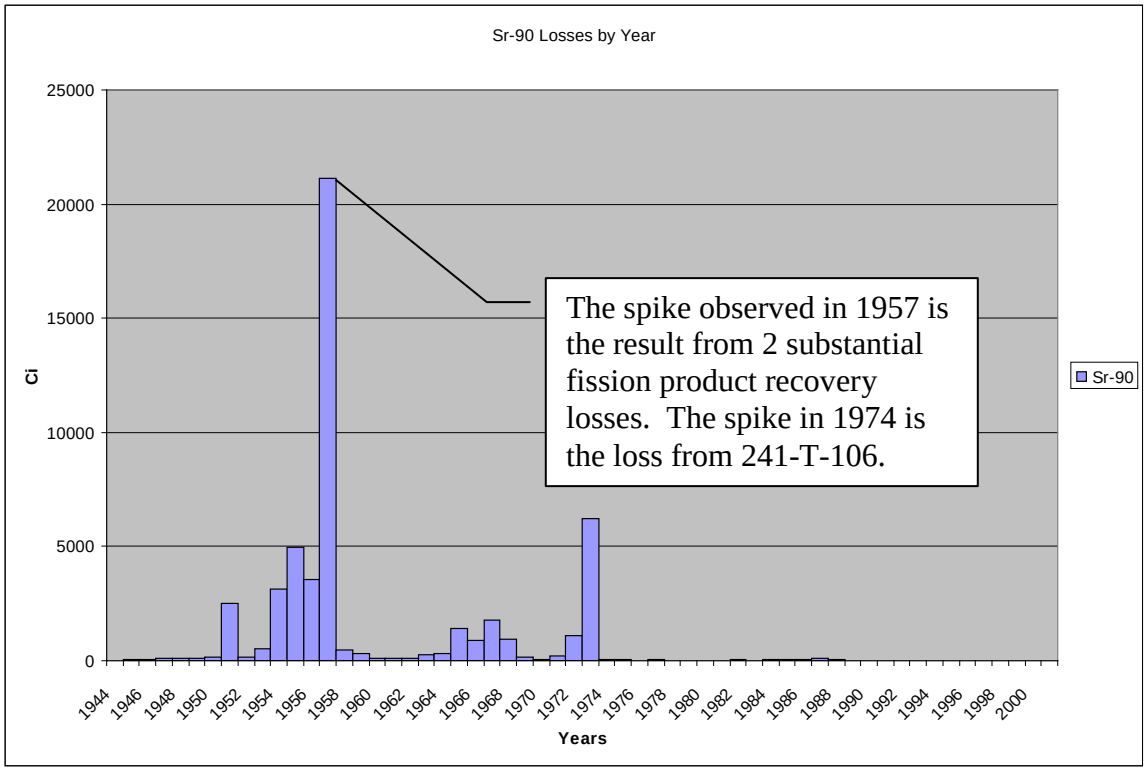


Figure 6-13. Annual Tc-99 Losses

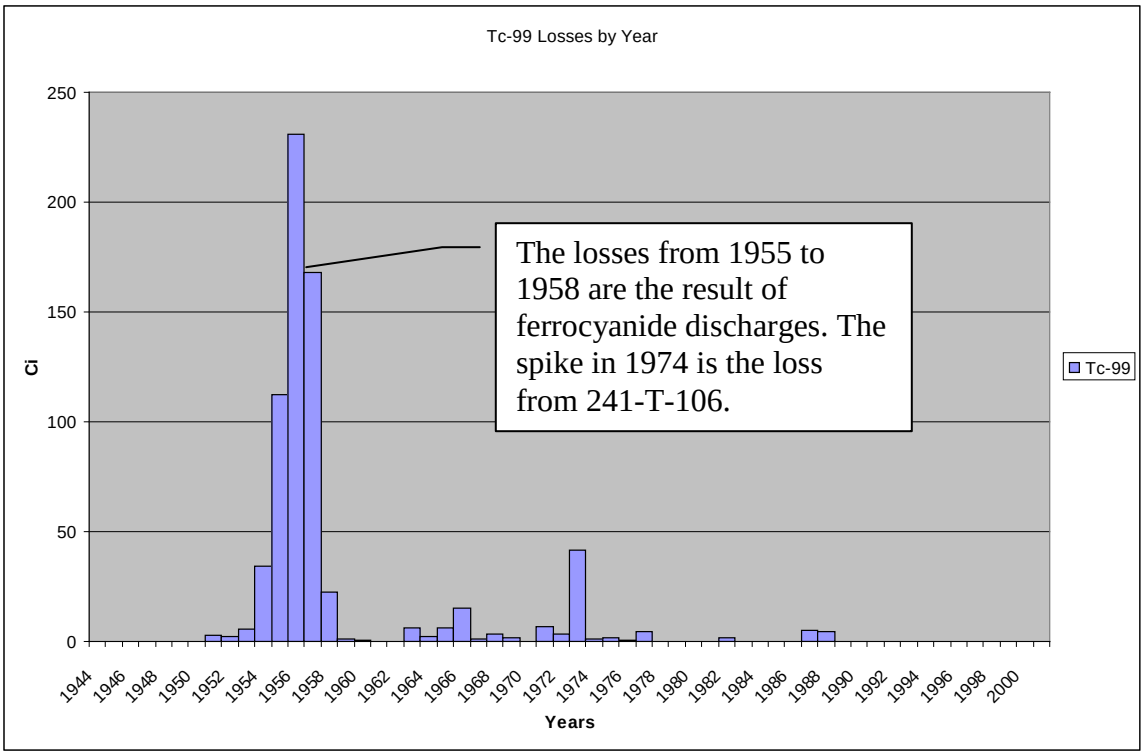


Figure 6-14. Annual I-129 Losses

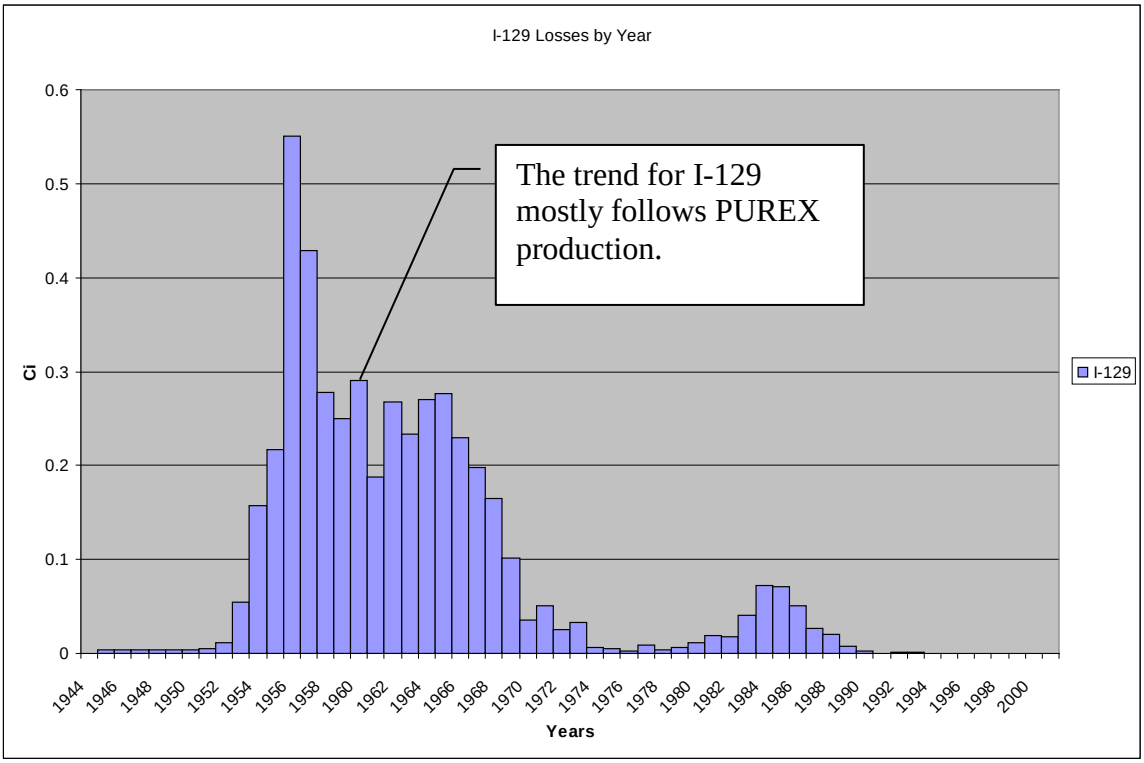


Figure 6-15. Annual Cs-137 Losses

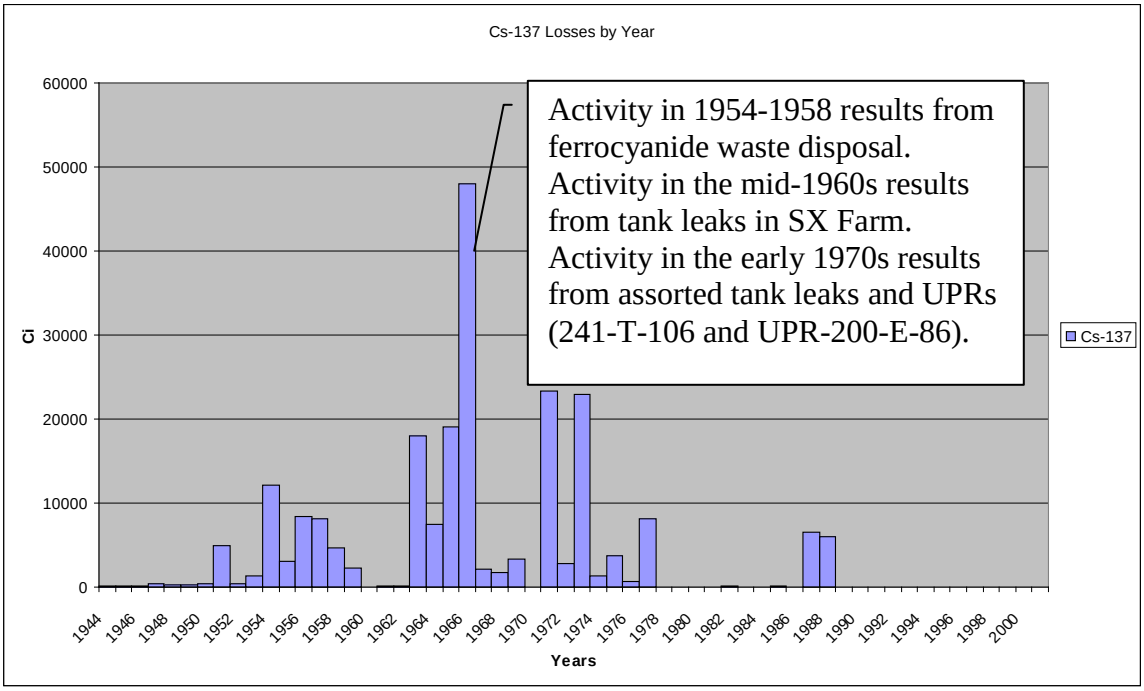


Figure 6-16. Annual Total Uranium Losses

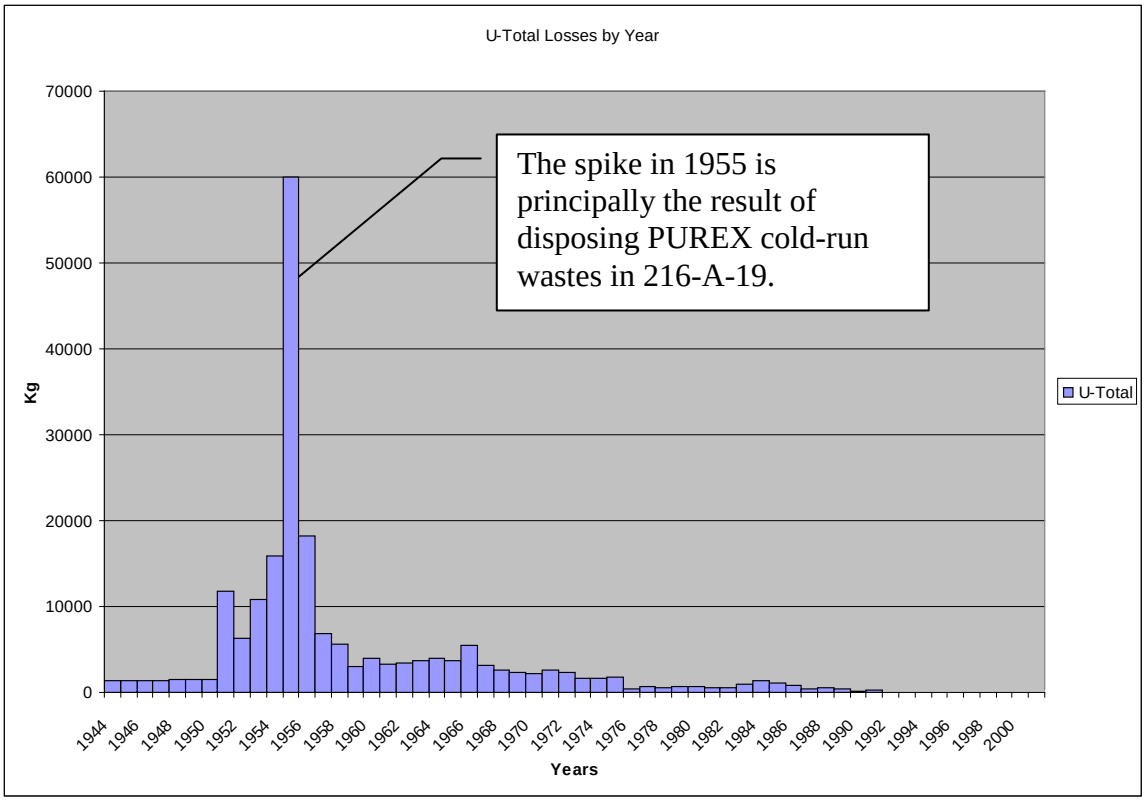


Figure 6-17. Annual Pu-239 Losses

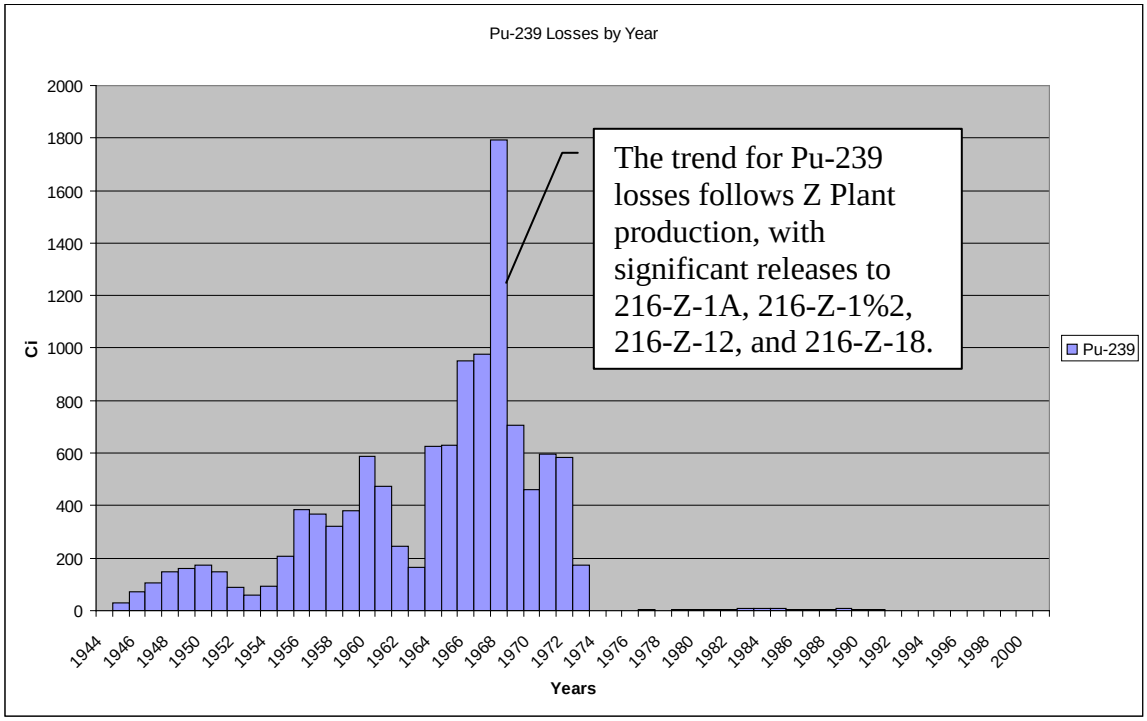


Figure 6-18. Annual Carbon Tetrachloride Losses

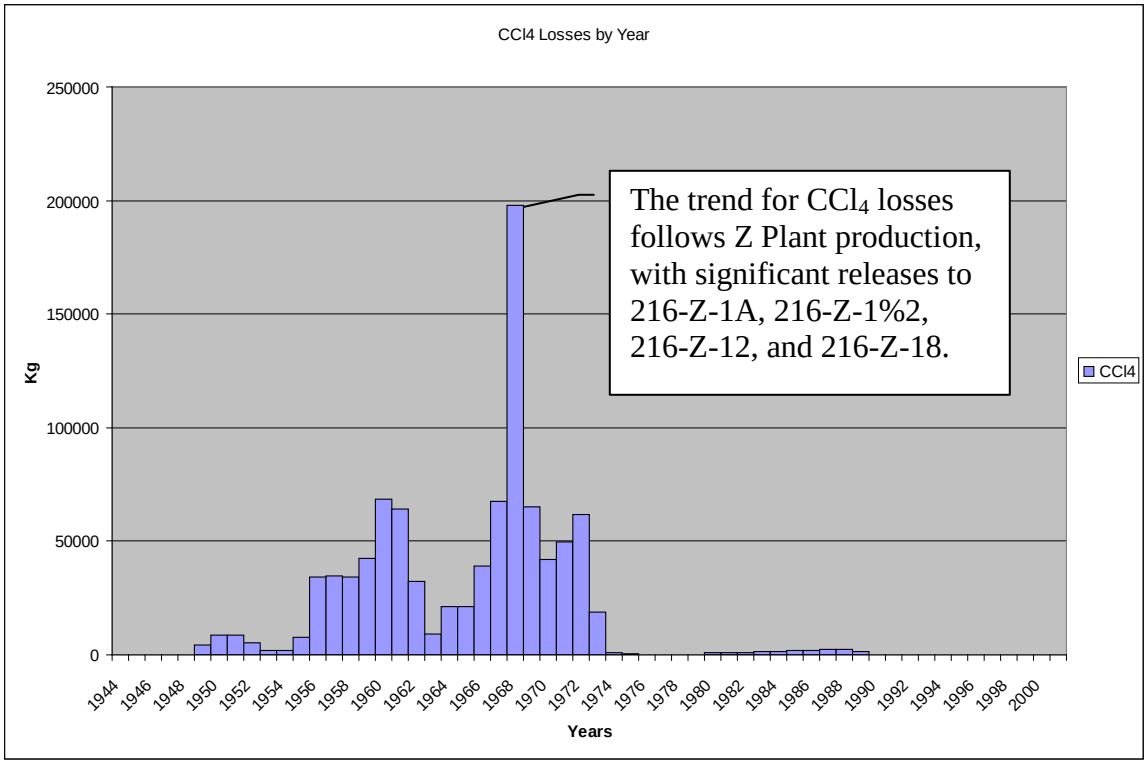
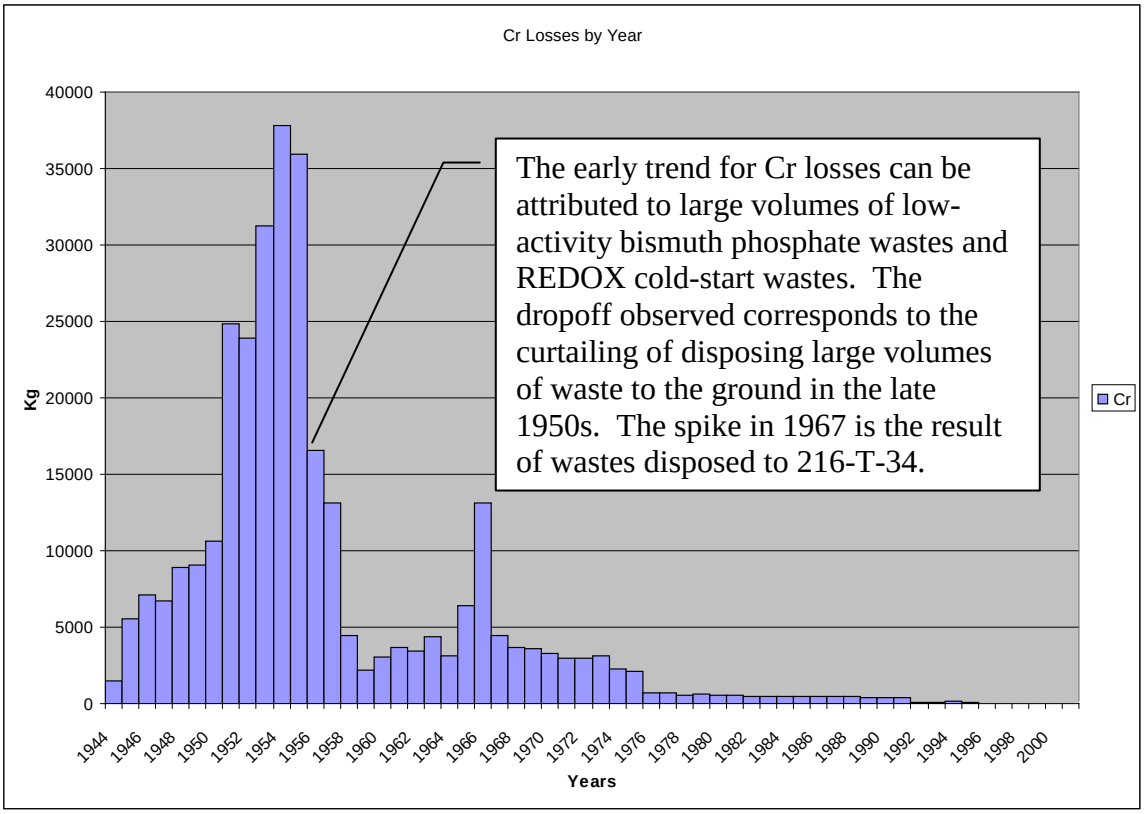


Figure 6-19. Annual Cr Losses



6.3 SECOND ORDER COMPARISONS

The following second-order comparisons are for the SAC analytes of interest by site as a percentage of inventory. Both absolute and relative inventory quantities are provided in Tables 6-20 to 6-28.

Table 6-20. Distribution of H-3 Inventory by Specific Site

Operable Unit	Site	H-3 Mean Inventory (Ci)	Percent of Total Inventory Lost
PUREX ZONE	216-A-10	5.78E+04	32.62%
200-E PONDS ZONE	216-A-8	2.46E+04	13.87%
200-E PONDS ZONE	216-B-3	2.01E+04	11.37%
PUREX ZONE	216-A-5	1.71E+04	9.64%
200-E PONDS ZONE	216-A-24	8.80E+03	4.97%
REDOX ZONE	216-S-7	8.38E+03	4.73%
T FARM ZONE	216-T-19	5.12E+03	2.89%
U PLANT ZONE	216-U-8	4.62E+03	2.61%
U PLANT ZONE	216-U-16	4.18E+03	2.36%
200-W PONDS ZONE	216-S-25	3.62E+03	2.05%
Top 10 Total Inv. (Ci)		1.54E+05	87.11%

Evaluating this table in conjunction with Table 6-10 above illustrates that two operable units are responsible for greater than 75% of the tritium inventory disposed. These waste streams and sites are logically predisposed to be elevated because they are the result of fuel and cladding dissolution operations. Because there is no practical segregation of tritium from the process water/condensate streams, once liberated and removed from the tank-canyon system, the tritium will principally reside in these separations process distillates/tank farm condensate wastes and relatively little of it will remain in the tanks.

Table 6-21. Distribution of Sr-90 Inventory by Specific Site

Operable Unit	Site	Sr-90 Mean Inventory (Ci)	Percent of Total Inventory Lost
UNASSIGNED 200 AREA	200-E-57	1.11E+04	21.48%
UNASSIGNED 200 AREA	200-E-56	7.38E+03	14.32%
T FARM ZONE	241-T-106	5.96E+03	11.56%
B FARM ZONE	241-BX-102	2.36E+03	4.58%
B FARM ZONE	216-B-7A%B	1.64E+03	3.17%
REDOX ZONE	216-S-7	1.47E+03	2.85%
B FARM ZONE	216-B-45	1.03E+03	2.00%
B FARM ZONE	241-BX-101	1.00E+03	1.94%
REDOX ZONE	216-S-1%2	9.59E+02	1.86%
B FARM ZONE	216-B-49	8.98E+02	1.74%
Top 10 Total Inv. (Ci)		3.38E+04	65.50%

In this case, for Sr-90, there were a select few waste sites that were highly enriched in Sr-90. However, these few tank leaks and unplanned releases represent a highly disproportionate amount of inventory compared to other more conventional sites, such as the ferrocyanide waste sites. From a chemical and physical standpoint, Sr-90 is relatively straightforward to control because of its solubility behavior (e.g., it is mostly insoluble in the waste streams) and is easily detected. Contamination control procedures in the tank-canyon system were rigorous about not allowing Sr-90 into the environment.

Table 6-22. Distribution of Tc-99 Inventory by Specific Site

Operable Unit	Site	Tc-99 Mean Inventory (Ci)	Percent of Total Inventory Lost
T FARM ZONE	241-T-106	3.74E+01	5.45%
NRDWL-BC CONTROL ZONE	216-B-14	3.29E+01	4.80%
NRDWL-BC CONTROL ZONE	216-B-18	3.24E+01	4.71%
NRDWL-BC CONTROL ZONE	216-B-52	2.61E+01	3.80%
B FARM ZONE	216-B-49	2.55E+01	3.71%
B FARM ZONE	216-B-46	2.55E+01	3.71%
NRDWL-BC CONTROL ZONE	216-B-15	2.40E+01	3.50%
B FARM ZONE	216-B-44	2.13E+01	3.10%
NRDWL-BC CONTROL ZONE	216-B-19	2.01E+01	2.93%
NRDWL-BC CONTROL ZONE	216-B-16	1.97E+01	2.87%
Top 10 Total Inv. (Ci)		2.65E+02	38.56%

Because Tc-99 is pervasive and soluble, most of the losses to the environment have been through disposal of bismuth phosphate-based wastes to the ground (e.g., ferrocyanide) and in a single-tank leak event, but the overall source term available for loss was relatively small. Where other high-level wastes were lost, most of the time they were not in volumes significant enough to impact inventory (Kincaid 2005; Appendix A). Most of the Tc-99 inventory remains in the Hanford Site high-level waste tanks.

Table 6-23. Distribution of I-129 Inventory by Specific Site

Operable Unit	Site	I-129 Mean Inventory (Ci)	Percent of Total Inventory Lost
PUREX ZONE	216-A-10	1.73E+00	36.78%
PUREX ZONE	216-A-5	9.63E-01	20.42%
REDOX ZONE	216-S-7	3.51E-01	7.45%
200-W PONDS ZONE	216-U-10	2.14E-01	4.53%
REDOX ZONE	216-S-1%2	1.36E-01	2.88%
PUREX ZONE	216-A-6	7.30E-02	1.55%
NRDWL-BC CONTROL ZONE	216-B-52	5.18E-02	1.10%
T PLANT ZONE	216-W-LWC	5.08E-02	1.08%
NRDWL-BC CONTROL ZONE	216-B-14	4.23E-02	0.90%
NRDWL-BC CONTROL ZONE	216-B-18	4.15E-02	0.88%
Top 10 Total Inv. (Ci)		3.66E+00	77.55%

Because I-129 was not measured routinely as an analyte in any process effluent, the SIM calibrated losses from waste disposal activity from environmental monitoring data (Kincaid 2004; Appendix A). From a process chemistry point of view, it is reasonable to place most of the losses of I-129 in certain acidic waste streams and condensates, but most of the I-129 inventory remains in the Hanford Site high-level waste tanks, albeit less than anticipated (Kupfer et al. 1999).

Table 6-24. Distribution of Cs-137 Inventory by Specific Site

Operable Unit	Site	Cs-137 Mean Inventory (Ci)	Percent of Total Inventory Lost
S-U FARM ZONE	241-SX-108	4.18E+04	18.78%
WTP-ETF-A-C FARM ZONE	UPR-200-E-86	1.98E+04	8.90%
S-U FARM ZONE	241-SX-107	1.79E+04	8.05%
S-U FARM ZONE	241-SX-115	1.49E+04	6.70%
T FARM ZONE	241-T-106	1.13E+04	5.07%
B PLANT ZONE	216-B-62	9.67E+03	4.35%
T FARM ZONE	241-TX-107	8.06E+03	3.62%
200-E PONDS ZONE	216-A-25	7.26E+03	3.26%
WTP-ETF-A-C FARM ZONE	241-A-103	6.53E+03	2.93%
S-U FARM ZONE	241-SX-104	5.93E+03	2.67%
Top 10 Total Inv. (Ci)		1.43E+05	64.33%

In this case, for Cs-137, there were a select few waste sites that were highly enriched in cesium, and these tank leaks and unplanned releases represent a highly disproportionate amount of inventory compared to other waste disposal sites. From a chemical and physical standpoint, Cs-137 is relatively tough to control because of its solubility behavior (e.g., it is mostly soluble in the aqueous waste streams), but it is easily detected. Thus, contamination control procedures in the tank-canyon system were rigorous about monitoring for and not allowing Cs-137 into the environment.

Table 6-25. Distribution of U-Total Inventory by Specific Site

Operable Unit	Site	U-Total Mean Inventory (kg)	Percent of Total Inventory Lost
200-E PONDS ZONE	216-A-19	4.34E+04	21.08%
UNASSIGNED 300 AREA	316-1	2.62E+04	12.70%
U PLANT ZONE	216-U-8	2.55E+04	12.38%
UNASSIGNED 300 AREA	316-2	1.94E+04	9.41%
B PLANT ZONE	216-B-12	1.51E+04	7.33%
200-E PONDS ZONE	216-A-25	1.22E+04	5.92%
B FARM ZONE	241-BX-102	1.01E+04	4.88%
U PLANT ZONE	216-U-12	6.46E+03	3.13%
PUREX ZONE	216-A-4	5.39E+03	2.61%
U PLANT ZONE	216-U-1%2	3.96E+03	1.92%
Top 10 Total Inv. (kg)		1.68E+05	81.36%

Significant losses for uranium are constrained to process cold start sites, where waste streams with unremoved particulate were allowed to be disposed; fuel rod production in the 300 Area, where a significant amount of uranium was left; and in the disposal of certain uranium recycle streams. From a chemical and physical standpoint, uranium is relatively easy to control because of its solubility behavior (e.g., it is insoluble in most of the waste streams, except the concentrated uranyl nitrate hexhydrate [UNH] waste). The 241-BX-102 event represents an anomaly in this group of sites, because most tank losses do not entrain particulate.

Table 6-26. Distribution of Pu-239 Inventory by Specific Site

Operable Unit	Site	Pu-239 Mean Inventory (Ci)	Percent of Total Inventory Lost
PFP ZONE	216-Z-1A	3.19E+03	27.06%
PFP ZONE	216-Z-12	2.48E+03	21.05%
PFP ZONE	216-Z-9	1.88E+03	15.97%
PFP ZONE	216-Z-18	1.77E+03	15.04%
PFP ZONE	216-Z-7	5.05E+02	4.28%
200-W PONDS ZONE	216-U-10	3.08E+02	2.62%
T FARM ZONE	216-T-7	2.36E+02	2.01%
PUREX ZONE	216-A-9	1.83E+02	1.56%
PFP ZONE	216-Z-1%2	1.48E+02	1.25%
B FARM ZONE	216-B-8	1.26E+02	1.07%
Top 10 Total Inv. (Ci)		1.08E+04	91.91%

For Pu-239, there were a few Z Plant waste sites that were very highly enriched in plutonium and these represent a highly disproportionate amount of inventory compared to other waste disposal sites. From a chemical and physical standpoint, losses of Pu-239 were relatively easy to control because of its solubility behavior in aqueous waste streams of the separation plants (e.g., it is mostly insoluble in those waste streams) and because it was the desired product, processes were optimized to capture as much of it as possible. However, it is difficult to detect as a result of surveillance, because it is an alpha emitter and the total alpha surveillance measurements are often confounded with americium.

Furthermore, the production situation was much different in Z Plant, where plutonium purification and recycling was occurring. The process solvent in use was carbon tetrachloride and plutonium is quite soluble in that; therefore, plutonium losses resulting from disposal of spent solvent to the cribs there were much more significant. Furthermore, because most of the fission products had been removed, there were fewer tell-tale signs for contamination control and surveillance. Although there were significant pressures to reclaim and minimize plutonium losses during the production mission, the losses that occurred in these streams and sites represent the nominal recovery process performance.

Table 6-27. Distribution of CCl_4 Inventory by Specific Site

Operable Unit	Site	CCl_4 Mean Inventory (kg)	Percent of Total Inventory Lost
PFP ZONE	216-Z-1A	3.07E+05	31.94%
PFP ZONE	216-Z-9	2.08E+05	21.70%
PFP ZONE	216-Z-18	1.92E+05	19.99%
PFP ZONE	216-Z-12	1.35E+05	14.07%
200-W PONDS ZONE	216-U-10	3.91E+04	4.07%
PFP ZONE	216-Z-1%2	3.80E+04	3.96%
PFP ZONE	216-Z-3	2.25E+04	2.34%
PFP ZONE	216-Z-21	7.92E+03	0.83%
200-E PONDS ZONE	216-B-3	4.68E+03	0.49%
200-E PONDS ZONE	216-A-25	2.20E+03	0.23%
Top 10 Total Inv. (kg)		9.56E+05	99.62%

There were a select few Z Plant waste streams that used carbon tetrachloride as the principal solvent instead of water, and although relatively small in volume, these streams and the sites to which they were disposed represent a highly disproportionate amount of CCl_4 inventory compared to the rest of the 200 Area waste disposal sites. A very small amount of CCl_4 was lost to the tank farm system from Z Plant and then processed through the evaporators.

Table 6-28. Distribution of Cr Inventory by Specific Site

Operable Unit	Site	Cr Mean Inventory (kg)	Percent of Total Inventory Lost
SEMIWORKS ZONE	216-C-1	5.77E+04	18.39%
REDOX ZONE	216-S-8	2.88E+04	9.17%
T FARM ZONE	216-T-7	2.81E+04	8.94%
UNASSIGNED 300 AREA	316-1	2.78E+04	8.86%
UNASSIGNED 300 AREA	316-2	2.03E+04	6.46%
B FARM ZONE	216-B-7A%B	1.16E+04	3.70%
WM ZONE	216-T-4A	1.14E+04	3.64%
T FARM ZONE	216-T-32	1.03E+04	3.28%
200-W PONDS ZONE	216-U-10	9.01E+03	2.87%
B FARM ZONE	216-B-8	6.23E+03	1.98%
Top 10 Total Inv. (kg)		2.11E+05	67.31%

The behavior of chromium is substantially different than the other analytes under review. Because it was a process chemical in the separation processes and also introduces itself as a corrosion product during operations, the distribution of chromium is not as driven by a few sites with highly elevated concentrations. It is more significantly influenced by low to modest levels of chromium coupled with significant volumes. The presence of the 300 Area fuel rod production sites is notable with respect to chromium and its relationship to uranium.

6.3.1 Global Second Order Comparisons

The second order comparisons present the results for each analyte on an individual basis, but at a consolidated level (e.g., over the entire operating history of the site). The results in Table 6-29 are presented in absolute percentage terms. Thus, for sodium, the top 10 sites contain 43% of the total sodium disposed in the 200 Area (and selected 300 Area sites) for the liquid waste sites, tank leaks, and unplanned releases; and the single site (216-T-7) contains 8% of the total sodium disposed to those categories of sites.

Table 6-29. Relationship of Top 10 Inventory Sites and Top Site Inventory to Overall Inventory in Percent. (3 Sheets)

Analyte	Top 10 Sites Percent of Total Inventory	Top Site	Single Site Percent of Total Inventory
Na	43.92%	216-T-7	8.05%
Al	97.91%	316-1	37.42%
Fe	69.35%	216-Z-12	14.35%
Cr	67.31%	216-C-1	18.39%
Bi	77.95%	216-T-7	24.04%
La	100.00%	216-B-5	49.80%
Hg	99.97%	216-Z-12	56.89%
Zr	69.63%	216-T-26	39.80%
Pb	98.55%	316-1	42.90%
Ni	53.40%	316-1	11.85%
Ag	93.63%	316-1	42.34%

Table 6-29. Relationship of Top 10 Inventory Sites and Top Site Inventory to Overall Inventory in Percent. (3 Sheets)

Analyte	Top 10 Sites Percent of Total Inventory	Top Site	Single Site Percent of Total Inventory
Mn	88.84%	216-B-3	16.24%
Ca	92.98%	216-B-3	40.64%
K	96.07%	216-Z-16	52.82%
NO_3	38.19%	216-T-7	7.32%
NO_2	91.36%	216-S-16P	24.28%
CO_3	97.48%	216-A-25	41.78%
PO_4	58.15%	216-U-10	25.92%
SO_4	78.62%	216-A-25	26.05%
Si	92.64%	216-A-25	33.07%
F	90.81%	216-Z-16	58.96%
Cl	77.59%	216-Z-16	26.92%
CCl_4	99.62%	216-Z-1A	31.94%
Butanol	99.62%	216-B-3	73.22%
TBP	97.30%	216-A-7	21.66%
NPH	96.96%	216-A-7	24.96%
NH3	90.92%	216-A-36B	53.91%
$Fe(CN)_6$	100.00%	216-T-26	85.73%
H-3	87.11%	216-A-10	32.62%
C-14	78.63%	216-B-3	50.28%
Ni-59	68.45%	241-SX-115	18.00%
Ni-63	67.77%	241-SX-115	17.61%
Co-60	35.71%	241-T-106	8.36%
Se-79	36.08%	241-T-106	5.41%
Sr-90	65.50%	200-E-57	21.48%
Y-90	65.49%	200-E-57	21.48%
Zr-93	47.90%	216-T-7	11.19%
Nb-93m	49.00%	216-T-7	11.65%
Tc-99	38.56%	241-T-106	5.45%
Ru-106	99.62%	216-A-10	62.35%
Cd-113m	36.43%	241-T-106	9.61%
Sb-125	58.45%	241-T-106	25.03%
Sn-126	37.77%	241-T-106	6.15%
I-129	77.55%	216-A-10	36.78%
Cs-134	72.18%	241-SX-108	17.44%
Cs-137	64.33%	241-SX-108	18.78%
Ba-137m	64.33%	241-SX-108	18.77%
Sm-151	33.76%	216-T-7	4.61%
Eu-152	41.49%	200-E-57	9.64%
Eu-154	41.44%	200-E-57	9.89%
Eu-155	41.88%	200-E-57	9.60%
Ra-226	41.80%	216-U-1%2	10.80%
Ra-228	90.95%	UPR-200-E-81	33.05%
Ac-227	40.55%	216-U-1%2	10.51%
Pa-231	61.16%	216-T-7	17.60%
Th-229	96.05%	216-U-12	89.42%
Th-232	97.70%	216-U-12	83.49%
U-232	99.16%	316-1	48.25%
U-233	99.28%	316-1	48.36%

Table 6-29. Relationship of Top 10 Inventory Sites and Top Site Inventory to Overall Inventory in Percent. (3 Sheets)

Analyte	Top 10 Sites Percent of Total Inventory	Top Site	Single Site Percent of Total Inventory
U-234	80.38%	216-A-19	19.67%
U-235	80.41%	216-A-19	20.48%
U-236	80.11%	216-A-25	15.68%
U-238	81.38%	216-A-19	21.12%
U-Total	81.36%	216-A-19	21.08%
Np-237	87.18%	216-Z-1A	23.02%
Pu-238	95.99%	216-Z-1A	37.55%
Pu-239	91.91%	216-Z-1A	27.06%
Pu-240	94.19%	216-Z-1A	32.92%
Pu-241	96.21%	216-Z-1A	38.35%
Pu-242	96.73%	216-Z-1A	38.77%
Am-241	97.55%	216-Z-12	29.65%
Am-243	98.13%	216-Z-12	48.24%
Cm-242	98.11%	216-Z-12	47.41%
Cm-243	99.13%	216-Z-12	48.72%
Cm-244	99.14%	216-Z-12	48.71%

Additionally, a site may have high [or the highest] inventories of several analytes, because this feature is not mutually exclusive. Table 6-30 illustrates which sites have several of the highest analyte inventories. This quantification of inventory does not incorporate the solid wastes buried at the Hanford Site, and thus, is an incomplete description, but it is a useful means of identifying specific sites of importance.

Table 6-30. Highest Analyte Inventory Membership Per Waste Site. (2 Sheets)

Waste Site	No. of Analytes	Analytes Where Site Has Single Largest Inventory
200-E-57	5	Eu-152, Eu-154, Eu-155, Sr-90, Y-90
216-A-10	3	H-3, I-129, Ru-106
216-A-19	4	U-234, U-235, U-238, U-Total
216-A-25	4	CO_3, Si, SO_4, U-236
216-A-36B	1	NH_3
216-A-7	2	NPH, TBP
216-B-3	4	Butanol, C-14, Ca, Mn
216-B-5	1	La
216-C-1	1	Cr
216-S-16P	1	NO_2
216-T-26	2	$Fe(CN)_6$, Zr
216-T-7	7	Bi, Na, Nb-93m, NO_3, Pa-231, Sm-151, Zr-93
216-U-1%2	2	Ac-227, Ra-226
216-U-10	1	PO_4
216-U-12	2	Th-229, Th-232
216-Z-12	7	Am-241, Am-243, Cm-242, Cm-243, Cm-244, Fe, Hg
216-Z-16	3	Cl, F, K

Table 6-30. Highest Analyte Inventory Membership Per Waste Site. (2 Sheets)

Waste Site	No. of Analytes	Analytes Where Site Has Single Largest Inventory
216-Z-1A	7	CCl_4, Np-237, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242
241-SX-108	3	Ba-137m, Cs-134, Cs-137
241-SX-115	2	Ni-59, Ni-63
241-T-106	6	Cd-113m, Co-60, Sb-125, Se-79, Sn-126, Tc-99
316-1	6	Ag, Al, Ni, Pb, U-232, U-233
UPR-200-E-81	1	Ra-228

6.3.1 Individual Second-Order Analyte Comparisons

Of the 179 sites in the Diediker (1999) database, not all of them consistently had inventory estimates for all of the analytes of interest. Thus, analytes were compared on an individual site-analyte basis. There are between 155 and 162 inventory estimates for each of the analytes in this set of sites. The remaining site-inventory combinations do not have comprehensive or consistent reference inventories, or have unacceptable discrepancies associated with the reference data; thus, they are not part of the evaluation process. Table 6-31 presents the individual quantitative comparison results for the selected analytes and the relative performance of the model for each site.

Table 6-31. Second-Order Comparison—Comparisons for Four Analytes by Specific Site. (5 Sheets)

Site	Sr-90	Cs-137	U-238	Pu-239	Number of Observations	Percent Values "in Range"
216-A-1	in range	in range	in range	in range	4	100%
216-A-10	SIM Low	SIM Low	in range	in range	2	50%
216-A-18	in range	in range	in range	in range	4	100%
216-A-19	in range	in range	in range	in range	4	100%
216-A-2	in range	in range	in range	in range	4	100%
216-A-20	in range	in range	in range	in range	4	100%
216-A-21	in range	in range	in range	in range	4	100%
216-A-24	SIM Low	in range	in range	in range	3	75%
216-A-25	in range	in range	in range	in range	4	100%
216-A-27	in range	in range	in range	in range	4	100%
216-A-28	--	--	in range	--	1	100%
216-A-3	in range	in range	in range	SIM Low	3	75%
216-A-30	SIM Low	SIM Low	SIM High	SIM High	0	0%
216-A-31	in range	in range	in range	SIM Low	3	75%
216-A-36A	in range	in range	in range	in range	4	100%
216-A-36B	in range	in range	in range	SIM Low	3	75%
216-A-37-1	SIM High	in range	in range	SIM High	2	50%
216-A-37-2	in range	SIM Low	in range	in range	3	75%
216-A-39	--	in range	--	--	1	100%
216-A-4	in range	in range	SIM High	SIM Low	2	50%

Table 6-31. Second-Order Comparison—Comparisons for Four Analytes by Specific Site. (5 Sheets)

Site	Sr-90	Cs-137	U-238	Pu-239	Number of Observations	Percent Values "in Range"
216-A-45	in range	SIM High	in range	in range	3	75%
216-A-5	in range	in range	in range	SIM High	3	75%
216-A-6	SIM Low	SIM Low	in range	in range	2	50%
216-A-7	in range	in range	in range	in range	4	100%
216-A-8	SIM Low	in range	in range	SIM Low	2	50%
216-A-9	in range	in range	SIM High	SIM High	2	50%
216-B-10A	in range	SIM High	in range	SIM Low	2	50%
216-B-10B	in range	in range	in range	in range	4	100%
216-B-11A%B	in range	in range	SIM Low	SIM Low	2	50%
216-B-12	in range	in range	in range	SIM Low	3	75%
216-B-14	in range	in range	in range	SIM High	3	75%
216-B-15	in range	in range	in range	SIM High	3	75%
216-B-16	in range	in range	in range	SIM High	3	75%
216-B-17	in range	in range	in range	in range	4	100%
216-B-18	in range	in range	in range	in range	4	100%
216-B-19	in range	in range	in range	SIM High	3	75%
216-B-20	in range	in range	in range	SIM High	3	75%
216-B-21	in range	in range	SIM Low	in range	3	75%
216-B-22	in range	SIM High	in range	SIM High	2	50%
216-B-2-2	--	--	--	--	Not quantified	--
216-B-23	in range	in range	in range	SIM High	3	75%
216-B-2-3	--	--	--	--	Not quantified	
216-B-24	in range	in range	in range	in range	4	100%
216-B-25	in range	in range	in range	SIM High	3	75%
216-B-26	in range	in range	SIM Low	SIM High	2	50%
216-B-27	in range	SIM High	in range	SIM High	2	50%
216-B-28	in range	SIM High	in range	SIM High	2	50%
216-B-29	in range	SIM High	in range	SIM High	2	50%
216-B-3	SIM High	SIM High	in range	in range	2	50%
216-B-30	in range	SIM Low	in range	SIM High	2	50%
216-B-31	in range	SIM High	in range	SIM High	2	50%
216-B-32	in range	in range	SIM High	SIM High	2	50%
216-B-33	SIM High	in range	in range	in range	3	75%
216-B-34	SIM High	SIM High	in range	SIM High	1	25%
216-B-35	in range	in range	in range	in range	4	100%
216-B-36	in range	in range	in range	in range	4	100%
216-B-37	SIM High	in range	SIM High	in range	2	50%
216-B-38	SIM Low	in range	in range	in range	3	75%
216-B-39	SIM High	SIM High	SIM High	in range	1	25%
216-B-40	in range	in range	in range	in range	4	100%

Table 6-31. Second-Order Comparison—Comparisons for Four Analytes by Specific Site. (5 Sheets)

Site	Sr-90	Cs-137	U-238	Pu-239	Number of Observations	Percent Values "in Range"
216-B-41	in range	in range	in range	SIM High	3	75%
216-B-42	in range	in range	SIM Low	in range	3	75%
216-B-43	in range	in range	in range	SIM High	3	75%
216-B-44	in range	in range	SIM High	SIM High	2	50%
216-B-45	in range	in range	SIM High	in range	3	75%
216-B-46	in range	in range	in range	in range	4	100%
216-B-47	in range	in range	SIM High	SIM High	2	50%
216-B-48	in range	in range	SIM High	SIM High	2	50%
216-B-49	in range	in range	in range	in range	4	100%
216-B-5	--	--	--	--	Not quantified	--
216-B-50	in range	in range	in range	in range	4	100%
216-B-52	SIM High	in range	SIM High	SIM High	1	25%
216-B-53A	SIM High	SIM High	in range	in range	2	50%
216-B-53B	in range	in range	in range	in range	4	100%
216-B-54	SIM High	SIM High	in range	in range	2	50%
216-B-55	in range	SIM Low	in range	in range	3	75%
216-B-57	SIM High	in range	in range	SIM High	2	50%
216-B-58	in range	in range	in range	in range	4	100%
216-B-59	SIM Low	SIM Low	--	--	0	0%
216-B-60	--	SIM Low	SIM Low	in range	1	33%
216-B-62	in range	in range	in range	in range	4	100%
216-B-63	SIM Low	in range	in range	in range	3	75%
216-B-7A%B	--	--	--	--	Not quantified	--
216-B-8	SIM High	SIM High	SIM High	SIM High	0	0%
216-B-9	SIM High	SIM High	SIM Low	in range	1	25%
216-C-1	in range	SIM High	in range	in range	3	75%
216-C-10	in range	SIM High	in range	in range	3	75%
216-C-3	in range	SIM High	SIM Low	SIM Low	1	25%
216-C-4	in range	in range	SIM Low	SIM Low	2	50%
216-C-5	SIM Low	in range	in range	in range	3	75%
216-C-6	in range	in range	SIM High	in range	3	75%
216-C-7	in range	in range	in range	in range	4	100%
216-C-9	in range	in range	in range	in range	4	100%
216-N-2	in range	in range	--	--	2	100%
216-N-3	in range	in range	--	--	2	100%
216-N-4	in range	SIM High	SIM Low	SIM Low	1	25%
216-N-5	in range	in range			2	100%
216-N-6	in range	SIM High	SIM Low	SIM Low	1	25%
216-N-7	in range	in range	--	--	2	100%
216-S-1%2	in range	in range	in range	in range	4	100%
216-S-10D	in range	SIM High	SIM High	SIM High	1	25%

Table 6-31. Second-Order Comparison—Comparisons for Four Analytes by Specific Site. (5 Sheets)

Site	Sr-90	Cs-137	U-238	Pu-239	Number of Observations	Percent Values "in Range"
216-S-11					Not quantified	
216-S-12	in range	in range	in range	in range	4	100%
216-S-13	SIM High	SIM High	in range	in range	2	50%
216-S-16P	in range	SIM High	in range	SIM Low	2	50%
216-S-17	in range	SIM High	SIM Low	SIM Low	1	25%
216-S-19	in range	in range	SIM Low	SIM Low	2	50%
216-S-20	SIM High	in range	SIM High	in range	2	50%
216-S-21	in range	in range	SIM Low	in range	3	75%
216-S-22	SIM Low	SIM Low	in range	in range	2	50%
216-S-23	SIM Low	SIM Low	in range	in range	2	50%
216-S-25	in range	in range	in range	SIM High	3	75%
216-S-26	SIM Low	SIM Low	in range	SIM Low	1	25%
216-S-3	in range	in range	in range	SIM Low	3	75%
216-S-5	in range	in range	in range	SIM Low	3	75%
216-S-6	SIM Low	SIM Low	in range	SIM Low	1	25%
216-S-7	in range	in range	in range	SIM High	3	75%
216-S-8	in range	in range	in range	in range	4	100%
216-S-9	in range	SIM Low	SIM High	in range	2	50%
216-T-1	SIM High	SIM High	SIM Low	in range	1	25%
216-T-12	SIM Low	in range	in range	SIM Low	2	50%
216-T-14	SIM High	in range	in range	in range	3	75%
216-T-15	SIM High	in range	in range	in range	3	75%
216-T-16	SIM High	in range	in range	in range	3	75%
216-T-17	SIM High	in range	in range	in range	3	75%
216-T-18	SIM High	in range	in range	SIM Low	2	50%
216-T-19	in range	SIM Low	in range	SIM High	2	50%
216-T-20	in range	in range	SIM Low	--	2	67%
216-T-21	SIM High	in range	in range	in range	3	75%
216-T-22	in range	in range	SIM High	in range	3	75%
216-T-23	SIM High	in range	SIM High	in range	2	50%
216-T-24	SIM High	in range	in range	in range	3	75%
216-T-25	SIM High	in range	SIM High	SIM High	1	25%
216-T-26	in range	in range	in range	SIM High	3	75%
216-T-27	SIM Low	SIM Low	in range	in range	2	50%
216-T-28	in range	in range	in range	in range	4	100%
216-T-3	--	--	--	--	Not quantified	--
216-T-32	--	--	--	--	Not quantified	--
216-T-33	in range	in range	in range	in range	4	100%
216-T-34	SIM Low	SIM Low	in range	in range	2	50%
216-T-35	SIM Low	SIM Low	in range	in range	2	50%
216-T-36	in range	in range	in range	in range	4	100%

Table 6-31. Second-Order Comparison—Comparisons for Four Analytes by Specific Site. (5 Sheets)

Site	Sr-90	Cs-137	U-238	Pu-239	Number of Observations	Percent Values "in Range"
216-T-4A	in range	in range	in range	SIM Low	3	75%
216-T-5	SIM High	in range	in range	in range	3	75%
216-T-6	--	--	--	--	Not quantified	--
216-T-7	--	--	--	--	Not quantified	--
216-T-8	SIM High	in range	in range	SIM Low	2	50%
216-U-1%2	in range	SIM Low	in range	SIM Low	2	50%
216-U-10	SIM High	SIM High	in range	SIM High	1	25%
216-U-12	in range	in range	in range	in range	4	100%
216-U-13	in range	in range	in range	in range	4	100%
216-U-15	SIM Low	in range	in range	in range	3	75%
216-U-16	in range	in range	SIM Low	SIM Low	2	50%
216-U-17	SIM Low	--	SIM Low	in range	1	33%
216-U-3	in range	SIM Low	in range	in range	3	75%
216-U-4A	in range	SIM Low	SIM Low	SIM High	1	25%
216-U-4B	SIM Low	SIM Low	--	in range	1	33%
216-U-5	in range	in range	in range	in range	4	100%
216-U-6	in range	in range	in range	in range	4	100%
216-U-8	in range	in range	in range	SIM Low	3	75%
216-W-LWC	in range	in range	in range	in range	4	100%
216-Z-1%2	in range	in range	SIM Low	in range	3	75%
216-Z-10	--	--	--	in range	1	100%
216-Z-12	SIM High	SIM High	in range	in range	2	50%
216-Z-16	in range	in range		in range	3	100%
216-Z-17	--	--	--	in range	1	100%
216-Z-18	--	--	--	in range	1	100%
216-Z-1A	SIM High	SIM High	in range	in range	2	50%
216-Z-20	in range	in range	--	in range	3	100%
216-Z-3	SIM High	SIM High	in range	SIM Low	1	25%
216-Z-4	in range	in range	in range	in range	4	100%
216-Z-5	in range	in range	SIM High	in range	3	75%
216-Z-6	SIM High	SIM High	in range	in range	2	50%
216-Z-7	in range	in range	SIM High	SIM High	2	50%
216-Z-8				in range	1	100%
216-Z-9	in range	in range	in range	in range	4	100%
UPR-200-W-38	in range	in range	in range	in range	4	100%
Legend	***Diediker "less thans"***					
	Other reference "less thans"					
	Corrected Diediker value					

Inspection of Table 6-32 illustrates the difficulties of evaluating the model with reference data values. Inconsistent treatment of "less than" values over time, lack of reference information, confounded tank and disposal site inventories, and various errors in the calculation of site inventories are not uncommon after reviewing the various source documents. The various discrepancies and inconsistencies that were observed and the method used to resolve/incorporate them in the comparison process are described in the table.

Table 6-32. Corrections or Modifications to the Discrepant/Inconsistent Database Values and the Application to the Comparison Process. (2 Sheets)

SAC Site Code	Sr90	Cs137	U238	Pu239
216-A-28	No reference data value	No reference data value		No reference data value
216-A-39	No reference data value		No reference data value	No reference data value
216-B-2-2	Consolidated inputs w/B-3	Consolidated inputs w/B-3	Consolidated inputs w/B-3	Consolidated inputs w/B-3
216-B-2-3	Consolidated inputs w/B-3	Consolidated inputs w/B-3	Consolidated inputs w/B-3; No reference data value	Consolidated inputs w/B-3; No reference data value
216-B-5	Removed from comparison because reference data included accumulation tank inventories	Removed from comparison because reference data included accumulation tank inventories	Removed from comparison because reference data included accumulation tank inventories	Removed from comparison because reference data included accumulation tank inventories
216-B-59			No reference data value	No reference data value
216-B-60	No reference data value			
216-B-7A%B	Removed from comparison because reference data included accumulation tank inventories	Removed from comparison because reference data included accumulation tank inventories	Removed from comparison because reference data included accumulation tank inventories	Removed from comparison because reference data included accumulation tank inventories
216-N-2			No reference data value	No reference data value
216-N-3			No reference data value	No reference data value
216-N-5			No reference data value	No reference data value
216-N-7			No reference data value	No reference data value
216-S-10D			Corrected reference data value; Maxfield (1979)	
216-S-11	Consolidated results w/S-10	Consolidated results w/S-10	Consolidated results w/S-10	Consolidated results w/S-10
216-S-16P			Corrected reference data value; Unsupported values and possible unit conversion and/or transcription errors observed in various references regarding 3160 kg of UNH solution	
216-S-25			Corrected reference data value; Maxfield (1979) provides range; used upper range value	
216-T-20				No reference data value

Table 6-32. Corrections or Modifications to the Discrepant/Inconsistent Database Values and the Application to the Comparison Process. (2 Sheets)

SAC Site Code	Sr90	Cs137	U238	Pu239
216-T-3	Removed from comparison because reference data included accumulation tank inventories	Removed from comparison because reference data included accumulation tank inventories	Removed from comparison because reference data included accumulation tank inventories	Removed from comparison because reference data included accumulation tank inventories
216-T-32	Removed from comparison because reference data included accumulation tank inventories	Removed from comparison because reference data included accumulation tank inventories	Removed from comparison because reference data included accumulation tank inventories	Removed from comparison because reference data included accumulation tank inventories
216-T-6	Removed from comparison because reference data included accumulation tank inventories	Removed from comparison because reference data included accumulation tank inventories	Removed from comparison because reference data included accumulation tank inventories	Removed from comparison because reference data included accumulation tank inventories
216-T-7	Removed from comparison because reference data included accumulation tank inventories	Removed from comparison because reference data included accumulation tank inventories	Removed from comparison because reference data included accumulation tank inventories	Removed from comparison because reference data included accumulation tank inventories
216-U-10			Corrected reference data value; DOE/RL 91-52 (DOE-RL 1992a)	
216-U-13	Corrected reference data value; Maxfield (1979)		Corrected reference data value; Maxfield (1979)	
216-U-17		No reference data value		
216-U-4B			No reference data value	
216-Z-1%2				Corrected reference data value; Unit conversion error (7000 g => ~434.5 Ci)
216-Z-10	No reference data value	No reference data value	No reference data value	
216-Z-16			No reference data value	
216-Z-17	No reference data value	No reference data value	No reference data value	
216-Z-18	No reference data value	No reference data value	No reference data value	
216-Z-1A				Corrected reference data value; Included inventory from Z-1AA, Z-1AB and Z-1AC
216-Z-20			No reference data value	
216-Z-8	No reference data value	No reference data value	No reference data value	
Legend				**No discrepancy identified**

Table 6-33 illustrates the strictest evaluation of the model by comparing the reference value with the computed interval range, with no allowances for the impact of less than values. The impact of the various “less than” inventories can be seen in the subsequent tables (Tables 6-34 and 6-35) where correction for the “less than” estimates are made (e.g., if the SIM value computed is strictly less than the reference value, it qualifies as being in range, ensuring logical consistency in evaluation). Furthermore, the observed SIM performance is significantly affected by the inconsistent treatment of “less than” values in the reference data. The comprehensive improvement in model performance from the no “less than values” corrected to all “less than values” corrected ranges from 10% to 14% depending on the analyte and, thus, cannot be ignored.

Table 6-33. Overall Analyte Comparisons by Site—Including "Less Than" Values

Initial output	*Sr-90*	*Cs-137*	*U-238*	*Pu-239*	*Total*
SIM low	39	40	34	47	160
in range	91	93	100	76	360
SIM high	31	29	21	37	118
Total compare	161	162	155	160	638
Percent in range	**57%**	**57%**	**65%**	**48%**	**56%**

Table 6-34. Overall Analyte Comparisons by Site—Correcting for Diediker (1999) "Less Than" Values

cCDI[1] *"less thans"*	*Sr-90*	*Cs-137*	*U-238*	*Pu-239*	*Total*
SIM low	28	30	25	38	121
in range	102	103	109	85	399
SIM high	31	29	21	37	118
Total compare	161	162	155	160	638
Percent in range	**63%**	**64%**	**70%**	**53%**	**62%**

Note: [1]**Diediker (1999); cCDI: nomenclature for compare Cumulative Decayed Inventory (cCDI)**

Table 6-35. Overall Analyte Comparisons by Site—Correcting for Diediker (1999) and Other Reference "Less Than" Values

All "less thans"	*Sr-90*	*Cs-137*	*U-238*	*Pu-239*	*Total*
SIM low	20	21	19	27	87
in range	110	112	115	96	433
SIM high	31	29	21	37	119
Total compare	161	162	155	160	638
Percent in range	**68%**	**69%**	**74%**	**60%**	**68%**

6.4 ANALYTE UNCERTAINTY EVALUATION

Results presented in this section contrast the membership and quantitative descriptions of two different categories of sites; the top ten sites as a function of inventory and the top ten sites as a function of uncertainty as quantified by RSD. Tables 6-36 to 6-53 illustrate the differences in the highest uncertainty sites and high inventory sites.

Table 6-36. H-3 Inventories by Sites with Significant Inventory

Analyte	Operable Unit	Site	Year	Mean	Std Dev	RSD
H-3	PUREX ZONE	216-A-10	Summation	5.78E+04	1.88E+04	32.56%
H-3	200-E PONDS ZONE	216-A-8	Summation	2.46E+04	1.06E+04	43.12%
H-3	200-E PONDS ZONE	216-B-3	Summation	2.01E+04	3.72E+03	18.46%
H-3	PUREX ZONE	216-A-5	Summation	1.71E+04	3.97E+03	23.26%
H-3	200-E PONDS ZONE	216-A-24	Summation	8.80E+03	3.43E+03	39.03%
H-3	REDOX ZONE	216-S-7	Summation	8.38E+03	2.43E+03	28.96%
H-3	T FARM ZONE	216-T-19	Summation	5.12E+03	1.76E+03	34.28%
H-3	U PLANT ZONE	216-U-8	Summation	4.62E+03	8.54E+02	18.48%
H-3	U PLANT ZONE	216-U-16	Summation	4.18E+03	4.53E+03	108.31%
H-3	200-W PONDS ZONE	216-S-25	Summation	3.62E+03	1.36E+03	37.57%

Table 6-37. H-3 Inventories by Sites with Largest Magnitude Uncertainty

Analyte	Operable Unit	Site	Year	Mean	Std Dev	RSD
H-3	PUREX ZONE	UPR-200-E-117	Summation	3.54E-03	7.00E-03	197.51%
H-3	UNASSIGNED 200 AREA 2	UPR-200-E-119	Summation	1.08E-06	2.11E-06	195.67%
H-3	B PLANT ZONE	UPR-200-E-85	Summation	4.92E-02	9.41E-02	191.30%
H-3	UNASSIGNED 200 AREA 2	UPR-200-W-127	Summation	9.66E-03	1.64E-02	169.35%
H-3	REDOX ZONE	UPR-200-W-32	Summation	7.69E-03	1.30E-02	168.52%
H-3	B PLANT ZONE	216-B-62	Summation	3.57E-01	5.75E-01	161.10%
H-3	B PLANT ZONE	216-B-60	Summation	4.60E-06	7.31E-06	158.81%
H-3	UNASSIGNED 200 AREA	200-E-107	Summation	7.28E-09	1.15E-08	157.46%
H-3	UNASSIGNED 200 AREA	200-E-54	Summation	5.45E-07	8.37E-07	153.68%
H-3	UNASSIGNED 200 AREA 2	UPR-200-E-141	Summation	6.50E-03	9.95E-03	153.23%

Table 6-38. Sr-90 Inventories by Sites with Significant Inventory

Analyte	Operable Unit	Site	Year	Mean	Std Dev	RSD
Sr-90	UNASSIGNED 200 AREA	200-E-57	Summation	1.11E+04	6.13E+03	55.38%
Sr-90	UNASSIGNED 200 AREA	200-E-56	Summation	7.38E+03	4.09E+03	55.39%
Sr-90	T FARM ZONE	241-T-106	Summation	5.96E+03	5.58E+03	93.74%
Sr-90	B FARM ZONE	241-BX-102	Summation	2.36E+03	9.78E+02	41.41%
Sr-90	B FARM ZONE	216-B-7A%B	Summation	1.64E+03	1.53E+03	93.60%
Sr-90	REDOX ZONE	216-S-7	Summation	1.47E+03	2.74E+02	18.64%
Sr-90	B FARM ZONE	216-B-45	Summation	1.03E+03	4.51E+02	43.87%
Sr-90	B FARM ZONE	241-BX-101	Summation	1.00E+03	1.06E+03	105.44%
Sr-90	REDOX ZONE	216-S-1%2	Summation	9.59E+02	2.14E+02	22.34%
Sr-90	B FARM ZONE	216-B-49	Summation	8.98E+02	4.13E+02	46.04%

Table 6-39. Sr-90 Inventories by Sites with Largest Magnitude Uncertainty

Analyte	Operable Unit	Site	Year	Mean	Std Dev	RSD
Sr-90	S-U FARM ZONE	241-S-104	Summation	1.02E+02	2.89E+02	283.72%
Sr-90	PFP ZONE	UPR-200-W-130	Summation	1.43E-10	3.02E-10	211.71%
Sr-90	PUREX ZONE	UPR-200-E-117	Summation	8.21E-01	1.58E+00	193.07%
Sr-90	B PLANT ZONE	UPR-200-E-85	Summation	6.24E+00	1.18E+01	189.26%
Sr-90	UNASSIGNED 200 AREA 2	UPR-200-E-119	Summation	2.50E-04	4.70E-04	188.00%
Sr-90	PFP ZONE	UPR-200-W-74	Summation	3.65E-17	6.12E-17	167.72%
Sr-90	UNASSIGNED 200 AREA 2	UPR-200-W-127	Summation	5.94E-11	9.67E-11	162.91%
Sr-90	B PLANT ZONE	216-B-60	Summation	2.28E-03	3.66E-03	160.50%
Sr-90	B PLANT ZONE	216-B-62	Summation	8.25E+01	1.31E+02	158.55%
Sr-90	T FARM ZONE	216-T-34	Summation	1.74E-01	2.68E-01	154.10%

Table 6-40. Tc-99 Inventories by Sites with Significant Inventory

Analyte	Operable Unit	Site	Year	Mean	Std Dev	RSD
Tc-99	T FARM ZONE	241-T-106	Summation	3.74E+01	4.01E+01	107.09%
Tc-99	NRDWL-BC CONTROL ZONE	216-B-14	Summation	3.29E+01	1.13E+01	34.23%
Tc-99	NRDWL-BC CONTROL ZONE	216-B-18	Summation	3.24E+01	1.54E+01	47.46%
Tc-99	NRDWL-BC CONTROL ZONE	216-B-52	Summation	2.61E+01	9.91E+00	37.99%
Tc-99	B FARM ZONE	216-B-49	Summation	2.55E+01	1.17E+01	45.91%
Tc-99	B FARM ZONE	216-B-46	Summation	2.55E+01	1.17E+01	45.86%
Tc-99	NRDWL-BC CONTROL ZONE	216-B-15	Summation	2.40E+01	8.59E+00	35.76%
Tc-99	B FARM ZONE	216-B-44	Summation	2.13E+01	6.95E+00	32.66%
Tc-99	NRDWL-BC CONTROL ZONE	216-B-19	Summation	2.01E+01	6.95E+00	34.61%
Tc-99	NRDWL-BC CONTROL ZONE	216-B-16	Summation	1.97E+01	7.29E+00	36.94%

Table 6-41. Tc-99 Inventories by Sites with Largest Magnitude Uncertainty

Analyte	Operable Unit	Site	Year	Mean	Std Dev	RSD
Tc-99	S-U FARM ZONE	241-S-104	Summation	3.96E-02	1.15E-01	290.51%
Tc-99	PFP ZONE	UPR-200-W-130	Summation	1.76E-11	3.86E-11	219.91%
Tc-99	B PLANT ZONE	UPR-200-E-85	Summation	3.57E-01	7.07E-01	198.04%
Tc-99	PUREX ZONE	UPR-200-E-117	Summation	2.39E-02	4.66E-02	194.70%
Tc-99	UNASSIGNED 200 AREA 2	UPR-200-E-119	Summation	7.25E-06	1.38E-05	190.00%
Tc-99	REDOX ZONE	UPR-200-W-32	Summation	1.56E-05	2.52E-05	161.80%
Tc-99	B PLANT ZONE	216-B-62	Summation	2.39E+00	3.84E+00	160.46%
Tc-99	B PLANT ZONE	216-B-60	Summation	8.14E-07	1.27E-06	156.36%
Tc-99	REDOX ZONE	UPR-200-W-87	Summation	1.53E-08	2.27E-08	147.96%
Tc-99	UNASSIGNED 200 AREA 2	UPR-200-E-40	Summation	5.33E-05	7.84E-05	146.96%

Table 6-42. I-129 Inventories by Sites with Significant Inventory

Analyte	Operable Unit	Site	Year	Mean	Std Dev	RSD
I-129	PUREX ZONE	216-A-10	Summation	1.73E+00	5.30E-01	30.56%
I-129	PUREX ZONE	216-A-5	Summation	9.63E-01	2.00E-01	20.80%
I-129	REDOX ZONE	216-S-7	Summation	3.51E-01	9.43E-02	26.84%
I-129	200-W PONDS ZONE	216-U-10	Summation	2.14E-01	3.45E-02	16.13%
I-129	REDOX ZONE	216-S-1%2	Summation	1.36E-01	4.61E-02	33.96%
I-129	PUREX ZONE	216-A-6	Summation	7.30E-02	1.48E-02	20.25%
I-129	NRDWL-BC CONTROL ZONE	216-B-52	Summation	5.18E-02	2.11E-02	40.72%
I-129	T PLANT ZONE	216-W-LWC	Summation	5.08E-02	3.23E-02	63.71%
I-129	NRDWL-BC CONTROL ZONE	216-B-14	Summation	4.23E-02	1.45E-02	34.31%
I-129	NRDWL-BC CONTROL ZONE	216-B-18	Summation	4.15E-02	1.97E-02	47.39%

Table 6-43. I-129 Inventories by Sites with Largest Magnitude Uncertainty

Analyte	Operable Unit	Site	Year	Mean	Std Dev	RSD
I-129	S-U FARM ZONE	241-S-104	Summation	5.56E-05	1.69E-04	304.94%
I-129	UNASSIGNED 200 AREA 2	UPR-200-E-119	Summation	3.92E-09	7.72E-09	196.75%
I-129	PUREX ZONE	UPR-200-E-117	Summation	1.27E-05	2.44E-05	191.77%
I-129	B PLANT ZONE	UPR-200-E-85	Summation	2.09E-04	3.88E-04	185.50%
I-129	B PLANT ZONE	216-B-62	Summation	1.29E-03	2.06E-03	160.03%
I-129	UNASSIGNED 200 AREA	200-E-107	Summation	2.34E-06	3.47E-06	148.02%
I-129	REDOX ZONE	UPR-200-W-87	Summation	2.39E-11	3.51E-11	146.87%
I-129	UNASSIGNED 200 AREA	200-E-54	Summation	6.42E-10	9.26E-10	144.33%
I-129	WTP-ETF-A-C FARM ZONE	241-A-103	Summation	5.28E-03	7.43E-03	140.70%
I-129	UNASSIGNED 200 AREA 2	UPR-200-E-81	Summation	2.38E-02	2.94E-02	123.40%

Table 6-44. Cs-137 Inventories by Sites with Significant Inventory

Analyte	Operable Unit	Site	Year	Mean	Std Dev	RSD
Cs-137	S-U FARM ZONE	241-SX-108	Summation	4.18E+04	3.89E+04	93.00%
Cs-137	WTP-ETF-A-C FARM ZONE	UPR-200-E-86	Summation	1.98E+04	2.32E+04	117.34%
Cs-137	S-U FARM ZONE	241-SX-107	Summation	1.79E+04	1.66E+04	92.94%
Cs-137	S-U FARM ZONE	241-SX-115	Summation	1.49E+04	1.13E+04	76.14%
Cs-137	T FARM ZONE	241-T-106	Summation	1.13E+04	5.94E+03	52.58%
Cs-137	B PLANT ZONE	216-B-62	Summation	9.67E+03	1.55E+04	160.20%
Cs-137	T FARM ZONE	241-TX-107	Summation	8.06E+03	9.43E+03	116.98%
Cs-137	200-E PONDS ZONE	216-A-25	Summation	7.26E+03	7.98E+03	109.89%
Cs-137	WTP-ETF-A-C FARM ZONE	241-A-103	Summation	6.53E+03	8.94E+03	136.86%
Cs-137	S-U FARM ZONE	241-SX-104	Summation	5.93E+03	5.19E+03	87.48%

Table 6-45. Cs-137 Inventories by Sites with Largest Magnitude Uncertainty

Analyte	Operable Unit	Site	Year	Mean	Std Dev	RSD
Cs-137	S-U FARM ZONE	241-S-104	Summation	1.19E+02	3.49E+02	294.55%
Cs-137	PFP ZONE	UPR-200-W-130	Summation	1.57E-10	3.55E-10	225.41%
Cs-137	PUREX ZONE	UPR-200-E-117	Summation	9.64E+01	1.88E+02	195.21%
Cs-137	UNASSIGNED 200 AREA 2	UPR-200-E-119	Summation	2.97E-02	5.69E-02	191.36%
Cs-137	B PLANT ZONE	UPR-200-E-85	Summation	3.73E+01	6.88E+01	184.60%
Cs-137	UNASSIGNED 200 AREA 2	UPR-200-W-127	Summation	1.47E-10	2.48E-10	168.29%
Cs-137	PFP ZONE	UPR-200-W-74	Summation	8.43E-17	1.41E-16	167.66%
Cs-137	B PLANT ZONE	216-B-62	Summation	9.67E+03	1.55E+04	160.20%
Cs-137	B PLANT ZONE	216-B-60	Summation	2.79E-03	4.36E-03	156.20%
Cs-137	UNASSIGNED 200 AREA	200-E-28	Summation	1.75E-03	2.66E-03	151.67%

Table 6-46. U-Total Inventory by Sites with Significant Inventory

Analyte	Operable Unit	Site	Year	Mean	Std Dev	RSD
U-Total	200-E PONDS ZONE	216-A-19	Summation	4.34E+04	3.94E+04	90.61%
U-Total	UNASSIGNED 300 AREA	316-1	Summation	2.62E+04	7.89E+03	30.14%
U-Total	U PLANT ZONE	216-U-8	Summation	2.55E+04	1.02E+04	40.12%
U-Total	UNASSIGNED 300 AREA	316-2	Summation	1.94E+04	6.57E+03	33.87%
U-Total	B PLANT ZONE	216-B-12	Summation	1.51E+04	7.21E+03	47.73%
U-Total	200-E PONDS ZONE	216-A-25	Summation	1.22E+04	3.72E+03	30.50%
U-Total	B FARM ZONE	241-BX-102	Summation	1.01E+04	5.38E+03	53.53%
U-Total	U PLANT ZONE	216-U-12	Summation	6.46E+03	2.86E+03	44.23%
U-Total	PUREX ZONE	216-A-4	Summation	5.39E+03	2.64E+03	49.01%
U-Total	U PLANT ZONE	216-U-1%2	Summation	3.96E+03	1.22E+03	30.77%

Table 6-47. U-Total Inventories by Sites with Largest Magnitude Uncertainty

Analyte	Operable Unit	Site	Year	Mean	Std Dev	RSD
U-Total	PFP ZONE	UPR-200-W-130	Summation	1.33E-06	4.10E-06	307.91%
U-Total	UNASSIGNED 200 AREA 2	UPR-200-W-103	Summation	3.29E-07	9.70E-07	294.62%
U-Total	PFP ZONE	UPR-200-W-74	Summation	4.69E-11	1.16E-10	247.43%
U-Total	UNASSIGNED 200 AREA 2	200-W-72	Summation	1.22E-05	2.66E-05	218.23%
U-Total	WTP-ETF-A-C FARM ZONE	241-A-103	Summation	6.44E-01	1.35E+00	210.44%
U-Total	UNASSIGNED 200 AREA 2	UPR-200-E-119	Summation	3.20E-06	6.35E-06	198.19%
U-Total	B PLANT ZONE	UPR-200-E-85	Summation	7.76E-02	1.53E-01	197.69%
U-Total	REDOX ZONE	UPR-200-W-32	Summation	2.83E-01	5.58E-01	197.05%
U-Total	PUREX ZONE	UPR-200-E-117	Summation	1.01E-02	2.00E-02	197.05%
U-Total	UNASSIGNED 200 AREA 2	UPR-200-W-127	Summation	9.91E-08	1.90E-07	192.17%

Table 6-48. Pu-239 Inventories by Sites with Significant Inventory

Analyte	Operable Unit	Site	Year	Mean	Std Dev	RSD
Pu-239	PFP ZONE	216-Z-1A	Summation	3.19E+03	2.31E+03	72.34%
Pu-239	PFP ZONE	216-Z-12	Summation	2.48E+03	8.92E+02	35.96%
Pu-239	PFP ZONE	216-Z-9	Summation	1.88E+03	5.93E+02	31.48%
Pu-239	PFP ZONE	216-Z-18	Summation	1.77E+03	1.05E+03	58.98%
Pu-239	PFP ZONE	216-Z-7	Summation	5.05E+02	8.64E+01	17.11%
Pu-239	200-W PONDS ZONE	216-U-10	Summation	3.08E+02	4.43E+02	143.60%
Pu-239	T FARM ZONE	216-T-7	Summation	2.36E+02	4.65E+01	19.69%
Pu-239	PUREX ZONE	216-A-9	Summation	1.83E+02	1.99E+02	108.51%
Pu-239	PFP ZONE	216-Z-1%2	Summation	1.48E+02	8.68E+01	58.74%
Pu-239	B FARM ZONE	216-B-8	Summation	1.26E+02	2.90E+01	22.98%

Table 6-49. Pu-239 Inventories by Sites with Largest Magnitude Uncertainty

Analyte	Operable Unit	Site	Year	Mean	Std Dev	RSD
Pu-239	PUREX ZONE	UPR-200-E-117	Summation	1.67E-03	4.05E-03	243.23%
Pu-239	B PLANT ZONE	UPR-200-E-85	Summation	1.26E-02	2.98E-02	236.38%
Pu-239	UNASSIGNED 200 AREA 2	UPR-200-E-119	Summation	5.12E-07	1.20E-06	235.04%
Pu-239	PFP ZONE	UPR-200-W-130	Summation	8.68E-06	1.97E-05	227.20%
Pu-239	UNASSIGNED 200 AREA 2	UPR-200-W-103	Summation	9.95E-01	2.19E+00	219.63%
Pu-239	B PLANT ZONE	216-B-62	Summation	1.68E-01	3.42E-01	203.32%
Pu-239	B PLANT ZONE	216-B-60	Summation	6.25E-02	1.27E-01	202.71%
Pu-239	UNASSIGNED 200 AREA 2	UPR-200-W-127	Summation	1.79E-07	3.57E-07	199.89%
Pu-239	UNASSIGNED 200 AREA 2	UPR-200-E-40	Summation	2.74E-04	5.21E-04	190.04%
Pu-239	PUREX ZONE	UPR-200-E-39	Summation	3.52E-03	6.65E-03	189.03%

Table 6-50. CCl_4 Inventory by Sites with Significant Inventory

Analyte	Operable Unit	Site	Year	Mean	Std Dev	RSD
CCl_4	PFP ZONE	216-Z-1A	Summation	3.07E+05	6.40E+04	20.89%
CCl_4	PFP ZONE	216-Z-9	Summation	2.08E+05	2.57E+04	12.34%
CCl_4	PFP ZONE	216-Z-18	Summation	1.92E+05	2.91E+04	15.16%
CCl_4	PFP ZONE	216-Z-12	Summation	1.35E+05	1.43E+04	10.59%
CCl_4	200-W PONDS ZONE	216-U-10	Summation	3.91E+04	1.26E+04	32.24%
CCl_4	PFP ZONE	216-Z-1%2	Summation	3.80E+04	4.87E+03	12.81%
CCl_4	PFP ZONE	216-Z-3	Summation	2.25E+04	2.82E+03	12.53%
CCl_4	PFP ZONE	216-Z-21	Summation	7.92E+03	7.93E+02	10.01%
CCl_4	200-E PONDS ZONE	216-B-3	Summation	4.68E+03	5.10E+02	10.90%
CCl_4	200-E PONDS ZONE	216-A-25	Summation	2.20E+03	2.67E+02	12.14%

Table 6-51. CCl_4 Inventory by Sites with Largest Magnitude Uncertainty

Analyte	Operable Unit	Site	Year	Mean	Std Dev	RSD
CCl_4	UNASSIGNED 200 AREA 2	UPR-200-W-103	Summation	1.29E+02	1.33E+02	103.42%
CCl_4	PFP ZONE	216-Z-20	Summation	2.90E+02	1.16E+02	39.94%
CCl_4	PFP ZONE	216-Z-8	Summation	3.62E+02	1.29E+02	35.57%
CCl_4	200-W PONDS ZONE	216-U-10	Summation	3.91E+04	1.26E+04	32.24%
CCl_4	PFP ZONE	216-Z-6	Summation	1.15E+00	3.68E-01	31.90%
CCl_4	PFP ZONE	216-Z-4	Summation	5.42E-01	1.72E-01	31.71%
CCl_4	PFP ZONE	216-Z-10	Summation	1.13E+01	3.59E+00	31.67%
CCl_4	PFP ZONE	216-Z-5	Summation	8.60E+00	1.82E+00	21.16%
CCl_4	PFP ZONE	216-Z-1A	Summation	3.07E+05	6.40E+04	20.89%
CCl_4	WM ZONE	216-T-4A	Summation	3.62E+02	6.09E+01	16.84%

Table 6-52. Cr Inventory by Sites with Significant Inventory

Analyte	Operable Unit	Site	Year	Mean	Std Dev	RSD
Cr	SEMIWORKS ZONE	216-C-1	Summation	5.77E+04	8.22E+03	14.24%
Cr	REDOX ZONE	216-S-8	Summation	2.88E+04	3.57E+03	12.40%
Cr	T FARM ZONE	216-T-7	Summation	2.81E+04	4.45E+03	15.87%
Cr	UNASSIGNED 300 AREA	316-1	Summation	2.78E+04	1.34E+03	4.83%
Cr	UNASSIGNED 300 AREA	316-2	Summation	2.03E+04	1.15E+03	5.68%
Cr	B FARM ZONE	216-B-7A%B	Summation	1.16E+04	1.89E+03	16.26%
Cr	WM ZONE	216-T-4A	Summation	1.14E+04	4.56E+02	4.00%
Cr	T FARM ZONE	216-T-32	Summation	1.03E+04	1.83E+03	17.80%
Cr	200-W PONDS ZONE	216-U-10	Summation	9.01E+03	6.37E+02	7.07%
Cr	B FARM ZONE	216-B-8	Summation	6.23E+03	1.17E+03	18.86%

Table 6-53. Cr Inventory by Sites with Largest Magnitude Uncertainty

Analyte	Operable Unit	Site	Year	Mean	Std Dev	RSD
Cr	UNASSIGNED 200 AREA 2	UPR-200-E-119	Summation	9.05E-05	1.06E-04	117.00%
Cr	PUREX ZONE	UPR-200-E-117	Summation	2.94E-01	3.42E-01	116.39%
Cr	UNASSIGNED 200 AREA 2	UPR-200-W-127	Summation	1.67E-04	1.92E-04	115.31%
Cr	B PLANT ZONE	UPR-200-E-85	Summation	4.08E+00	4.69E+00	115.17%
Cr	T PLANT ZONE	UPR-200-W-98	Summation	6.02E-02	6.93E-02	115.07%
Cr	UNASSIGNED 200 AREA 2	UPR-200-W-24	Summation	2.51E-02	2.87E-02	114.54%
Cr	B PLANT ZONE	UPR-200-E-1	Summation	7.30E+00	8.32E+00	113.98%
Cr	B PLANT ZONE	UPR-200-E-77	Summation	6.33E-03	7.06E-03	111.37%
Cr	PFP ZONE	UPR-200-W-130	Summation	4.12E-05	4.51E-05	109.50%
Cr	UNASSIGNED 200 AREA 2	UPR-200-W-102	Summation	9.38E+00	9.63E+00	102.71%

As can be observed from these comparisons, the sites with significant inventory and the sites with highly uncertain inventories (with a couple of exceptions) have very few members in common. This outcome is expected because there are known differences in the number and

quality of assumptions involved in calculating specific site inventories and these factors are at work in the SIM calculations of uncertainty.

Sites with highly uncertain inventories have features that tend to increase uncertainty, and they can impact each other synergistically, magnifying their combined effects. These uncertainty magnifying features can include:

- Relatively small, asymmetric volume distributions with zero as a lower bounding condition, broadening the volume uncertainty;
- Large numbers of contributing waste streams of small or similar volumes, but substantially different compositions (observed in certain tank leak descriptions), potentially smearing the effect on calculating mean inventory values; and
- Unplanned release events with highly uncertain volume bases.

In contrast, sites with significant inventory have features that tend to reduce uncertainty, however, that uncertainty can still be large. Sites with significant inventory have uncertainty reducing features such as:

- Known volumes of nominal variation, constraining the volume uncertainty, and
- One (or very few) waste stream(s) of consequence received, effectively dictating the inventory behavior.

For both categories of sites, there is no difference associated with the individual stream compositions—the uncertainties for concentration and density are identical, and thus, there are no discriminators on that basis.

The conditions in the highly uncertain sites interact to a significant degree and result in the substantial difference observed in uncertainty between the sites with significant inventory and elevated uncertainty. Thus, the SIM outputs are illustrating the difference between the quality and number of assumptions associated with the types and amounts of waste disposed to these two categories of sites (e.g., the highly uncertain sites often have RSDs over three times as large as the high inventory sites).

Waste streams that contribute significant amounts of a particular analyte can dampen the impact on uncertainty as a function of volume. Thus, waste streams that have a single dominating feature or impact on a waste site inventory can overwhelm any inventory/uncertainty contribution from a minor contributor; however, sites with a large number of relatively small contributors of similar magnitudes can increase the observed uncertainty. Therefore, this effect is generally observed in tank leaks.

7.0 CONCLUSIONS

SIM Rev. 1 provides estimates of the amounts and uncertainties associated with the contamination associated with the liquid waste disposal sites, unplanned releases, and tank leaks. This information leads to more effective use and application of remediation resources by allowing risk-based priorities to be established. Because of the modeling assumptions, the resulting output distributions were relatively simple—skewed, non-negative, and monomodal, each with a well-defined central maximum. More complicated behavior is possible for these model inputs (and outputs); however, the assumptions for the contaminants used in SIM are considered a practical compromise in appropriately describing uncertainties associated with Hanford Site waste management and disposal activities at a reasonable level of resolution.

7.1 GENERAL OBSERVATIONS REGARDING SIM

This modeling effort can provide valuable insight to the quantity and uncertainty associated with contaminated soil inventories at the Hanford Site, especially with regard to particular locations. However, it does not result in a technically defensible model if all that SIM does is parrot the reference values in a "just so story" (i.e., lacking independent empirical support). In the case of SIM, multiple lines of reasoning are used to support the model and demonstrate that a reasonable and consistent set of estimates are obtained. Those multiple lines of reasoning include (1) ~70% of the record/best-estimate values of disposal inventory for selected analytes lie within the uncertainty range predicted by SIM; (2) these results are routinely obtained using waste stream definitions based on a independently derived separations process model; and (3) available field evidence of contamination in the subsurface environment at the Hanford Site suggests that SIM provides a reasonable representation of the inventories and uncertainties. Investigating, correcting, and/or reconciling disagreements between modeling results and reference values can be useful to the process of quantifying uncertainty and reducing error with regard to inventory.

Although approximately 70% the selected analyte results were found to be within the 0.5 to 99.5 percentile range, this metric may be considered too generous to be considered agreement between SIM and the reference data for certain purposes. Further evaluations using narrower criteria may be justified to better describe model performance. Currently, the methods and assumptions used to represent the mean values and evaluate uncertainties in this revision of the model are considered coarse but realistic. In evaluating the data, the size of the uncertainties associated with these estimates are significant, spanning in some cases an order of magnitude. This condition does not necessarily represent a deficiency in the data; all that can be inferred is that the system has a substantial amount of intrinsic uncertainty and that any decisions made must take this feature into account.

If these magnitude uncertainties are unacceptable for making decisions, there are options that can be taken to improve the situation. In this case, one could either more closely quantify and reduce the range of the input uncertainties or better represent the uncertainties associated with the reference data so as not to prejudice the user's perception regarding the degree of certainty with regard to the reference data. These options for improvement could be implemented by

introducing correlations and additional distributions as part of a refined ORIGEN2 run to better quantify production uncertainty estimates, quantifying uncertainties around the reference values using historical information, or changing the uncertainty basis to better reflect the influence of solubility behavior.

Model assumptions, constraints associated with computer software coding, and the number of trials performed in the analysis removed many of the irregularities associated with the individual process batches and smoothed the variation observed in the source documentation. The principal factor influencing the model output is the degree to which reliable quantitative descriptions could be provided for the inputs. Sparse data with broad uncertainties used to quantify analyte behavior, or where simple distributional assumptions were used to quantify analyte behavior, were the largest contributors to uncertainty in the estimated inventories. This condition is especially true for individual realizations (e.g., annual results) for several analytes in SIM, in light of the large production uncertainties derived from the ORIGEN2 output. However, the uncertainties at more consolidated levels of evaluation (e.g., total inventory over operating history) were better behaved and did not have as widely variable spans as was observed at the individual year level.

Pareto-style behavior is routinely observed for inventory. The inventories for various analytes in the vadose zone are very highly skewed towards a select number of sites/operable units, and this behavior is a direct outcome of the evolution of waste management practices at the Hanford Site. Often waste streams with particular compositions were confined to a certain geographical area or set of disposal sites. This selectivity provided for a small number of sites containing the significant majority of a number of analytes of interest. The top ten sites by inventory for a particular analyte can generally account for 39% to 100% of the total mass/activity for that analyte calculated for this set of sites. Furthermore, sites with a significant inventory of a particular analyte are not mutually exclusive with regard to the amounts of other analytes. This behavior leads to a small subset of sites that would be particularly attractive from a risk-managed remediation perspective in order to optimize available resources (i.e., a small number of high inventory/risk sites).

7.2 PHYSICAL AND CHEMICAL ASSUMPTIONS REGARDING SIM WASTE STREAM BEHAVIOR

The physical and chemical assumptions regarding analyte concentrations have the greatest impact on inventories. Inventories of analytes that were disproportionally lost to the environment could be considered in three different categories:

- Those analytes that could be considered process water impurities and are principally influenced by overall water volume, such as calcium or sulfate. These inventories scale almost directly with volume and are not necessarily related to the chemical processes at the Hanford Site.

- Highly soluble and pervasive analytes such as sodium, nitrate, and chloride have significantly greater losses and are influenced by a combination of volume, composition, and solubility.

- Certain process-specific waste streams were highly enriched in particular analytes (e.g., Z Plant waste for plutonium and carbon tetrachloride). Although the volume of these wastes was relatively low, they represent the majority of the source term observed for these analytes. This feature is also evident when evaluating tank leak and unplanned release losses.

7.3 CONCLUSIONS REGARDING SIM ASSUMPTIONS DESCRIBING RADIONUCLIDE DISTRIBUTIONS

Both sample data and process engineering documentation show that there are a wide variety of concentrations and uncertainty behavior for each analyte as a function of both time and separation process. Because of the confounded and incomplete description of the waste being disposed (or escaping) to the environment, numerous assumptions regarding the amount, composition, and distribution of the wastes being discharged/lost were necessary. Principal among them was the mass-balance boundary condition that was imposed as a model requirement.

The mass balance boundary condition is important to consider when evaluating model output. There are two conventional applications of the mass-balance boundary condition in SIM. The first application is that the input waste streams are initially mass and charge balance as a function of the mean values. In SIM, each separations plant has its own separate global radionuclide inventory from which to derive losses that is internally conserved and consistent, minimizing the potential for confounding and temporal "cross-talk" in the results. Considering each separation process as an independent contributing entity, using the ORIGEN2 values for total reactor yield, the amount of fuel processed through each chemical processing plant, and the SIM estimates, corrected for decay, a loss fraction can be calculated.

This aspect was important for evaluating the REDOX or PUREX process effluents, because those systems were nearly closed (e.g., the wastes processed through these systems were placed in the tanks and certain of the radionuclides were often reclaimed/extracted and not deliberately disposed to the ground). When viewed in context, the overall losses of contaminated material from the tank-canyon system were very small and most process chemicals used at the Hanford Site were retained by the tank-canyon system. The active waste management, processing, and surveillance measures used to extract and retain radionuclides appear to have worked very well.

The second application of the mass balance boundary is that the mean SIM values for a particular analyte summed over all disposal sites must be less than or equal to the total losses of that analyte from the tank-canyon system. Because the probability distributions functions applied to the inputs are currently left unconstrained and each analyte is treated as an independent variable, summing extreme values (such as using all 90^{th} percentile values) for a particular analyte over all disposal sites to derive a global inventory will result in an unrealistic soil inventory estimate for that analyte. Because of the constrained source terms (both overall and for each separation

process), if an extremely high value is selected for a site or a series of sites, the availability of that analyte is diminished for the remaining sites, and there needs to be a concomitant number of sites with extremely low inventories of that analyte to maintain the mass conservation boundary.

7.4 SPECIFIC OBSERVATIONS REGARDING BEHAVIOR OF SAC ANALYTES

Volume disposed to a particular site can be seen to play a significant role with regard to inventory; however, for several analytes, there are other factors at work. Particularly, certain specific events (e.g., 241-BX-102), solubility considerations (e.g., H-3), disposal timing (e.g., Tc-99), reprocessing/recycling activity (e.g., Cs-137, Sr-90, Pu-239) or characteristics of the waste type (e.g., ferrocyanide scavenged waste) can be shown to impact particular contributions to vadose zone inventory more significantly than total volume, and thus, the assumption of a zero-order inventory model is not appropriate.

The tritium loss to total ratio is unusual in many respects. Unlike most other analytes, this analyte inventory is significantly influenced by its volatility. The tank-canyon system was designed to confine contamination, especially particulates. However, tritium was mostly lost as a vapor/condensate. Because there is no simple means of segregating the tritium from the process solution, and because evaporation was routinely used in reducing waste volume both in the separations processes and in the tank farms, the process condensate cribs that were direct reductions of high-level waste will have substantial tritium inventory and these inventories are expected to scale with the volume of waste evaporated. Therefore, most of the tritium (>90%) produced was lost from evaporation and allocated as a function of the waste high-level waste condensate discharged. Thus, most of the tritium produced was lost from the tank-canyon system to the ground, and it is one analyte whose global vadose zone inventory is anticipated to greatly exceed the global tank inventory because of its volatility. In addition, this analyte's source term is highly uncertain because of its dependence on the presence of an unquantified lithium impurity in the fuel cladding as part of the reactor production calculations (Higley 2003).

The I-129 loss ratio is a function of using environmental surveillance data and additional engineering judgment to estimate the source term for that analyte. Radioiodine was not typically measured in any process effluent, and thus, its estimated losses are determined using other means. Additionally, from a process chemistry perspective, the release of I-129 in acidic process condensate waste streams is understandable, because the analyte would be more soluble and mobile under those conditions.

The Tc-99 and other isotope inventories are significantly constrained because most (>70%) of the irradiated fuel was processed through PUREX, and the amounts of high-level process waste deliberately discharged to the soil were curtailed through most of PUREX's operating history. The most significant contribution of Tc-99 and these several other isotopes to the vadose zone are from the disposal of ferrocyanide waste. The entire production of Tc-99 throughout the bismuth phosphate production regime responsible for that source was less than 1,200 Ci in total, with similarly modest amounts for the other radionuclides produced at that time. Thus, the inventory that could be lost to the vadose zone would be relatively small. However, that does make the minor (from a global volumetric standpoint) losses from ferrocyanide waste disposal,

tank leaks, and unplanned releases relatively significant from an inventory perspective because of the types and concentrations of isotopes in those wastes.

Uranium was a special case in many respects; the 241-BX-102 event and direct disposal of cold-run waste disproportionately affected the loss to total ratio. Furthermore, the fuel fabrication activities in the 300 Area had very little information regarding the isotopic profile of the uranium available (both recycled and natural uranium were used), and uranium was often present when discharged to tank farms as a transiently soluble species. Because the ORIGEN2 values do not include the uranium inventory associated with the cold-run process waste, using those values as a basis for comparison does not represent the conditions in the tanks or the loss ratio in the vadose zone correctly.

Transuranic actinide loss-to-total ratios (including Pu-239) were relatively high across the board. This behavior was expected because it reflects several different modeling assumptions and boundary conditions. Although there were no entrained particulates in most of these waste streams, the impact of Z Plant losses and the differences in processing Z Plant waste versus the other separations plants significantly increased their contribution to soil inventory. The disposal of highly Pu-contaminated carbon tetrachloride solutions, resulting from recycle, rework, and process finishing, to specific sites in 200 West is significantly different from the separations plants in relationship to the source term. However, in the losses from the separation plants and tank farms directly, the transuranic losses are very low, reflecting their low solubility and the operational loss minimization prerogatives for these analytes in these facilities.

Laboratory testing may be needed to better quantify the solution behavior of uranium and plutonium under disposal conditions and volume percent solids in the waste streams. The mean isotopic distribution for plutonium and uranium was often derived using total alpha and uranium process engineering data and was allocated using the ORIGEN2 isotopic divisions for a particular processing regime. The degree of uncertainty acceptable in the SAC modeling effort will dictate if additional laboratory study is necessary or if more narrowly derived production uncertainties, specific to particular waste types are needed to better define the input uncertainty parameters for uranium, plutonium, or any other analyte of interest. The modular design of the model allows for identifying and quantifying individual contributions to uncertainty, allowing for modification and refinement where appropriate.

Where significant differences in RSDs for specific analytes were observed between liquid waste disposal sites/unplanned releases and tank leaks, the complexity of the tank leak composition is thought to be the significant contributor to uncertainty. The liquid waste disposal sites/unplanned releases consist of very limited numbers of waste streams, generally two to three waste streams are used to define the inventory for a site (although for these categories, the maximum is 31). Additionally, the waste streams in many cases do not differ much in composition for the analytes being evaluated, further constraining the uncertainty behavior for these two categories. However, because the tank leaks can consist of simultaneous linear combinations of numerous different waste streams (in this case, 44 is the maximum) with widely varying compositions and uncertainties, this very complex waste description has the potential to have waste input descriptions that would be more appropriately described as bi-modal or multi-modal. Instead, these components are combined together in a waste stream that results in a very

loosely defined mean or median and large uncertainty spanning several different ranges. This representation of the tank leak waste stream results in much larger composite analyte RSDs, even though the overall range of the individual waste stream component uncertainties was not affected.

7.5 REFERENCE DATA LIMITATIONS, CONFLICTS, AND ANOMALIES

The use of tank data or other historical process data in modeling was evaluated closely for appropriateness in each potential application in SIM. The effects of time and waste management operations have compromised much of the contemporary tank waste composition data for use in this modeling effort; thus, direct use of current tank sampling data is extremely limited. Furthermore, many of the waste streams disposed to the ground were never introduced to the tanks. Some closely followed analytes (e.g., Cs-137, Sr-90, Pu-239, etc.) have a long documented history of surveillance measurement. These results are sometimes incorporated directly as part of the model input definition process. The surveillance data-based analyte measurements (concentrations and/or inventories) are also used in a comparison with model outputs in a subsequent verification analysis.

The extensive use of the HDW Model (Higley et al. 2004) and latest ORIGEN2 output (Watrous et al. 2002) is a potential limitation on SIM as well. Although the sources, methods, and assumptions used in developing these models and their outputs are conventionally accepted and have gone through extensive review and analysis, there are inherent limitations on their performance as well. These limitations are discussed in detail in Higley et al. (2004). Additional problems associated with the reference data are that it is partially censored (certain data remain classified and unavailable), intermittent as a function of time (the type of data collected and the associated rigor is not consistent), and not comprehensive in scope (analytical results are present as a function of their level of management or process control interest at the time). Finally, because there is no independent source of comprehensive field data for comparison, validation of SIM is not possible at this time.

In many cases, the observed discrepancies between SIM estimates and the reference values result as a function of the smoothing assumptions used to develop general waste stream descriptions (composition and uncertainties) or may be attributable to one or more actions as a function of processing or human error within operations (e.g., dilution, rework, mixing, documentation error, process excursion, or separation and removal of analytes). The site- or batch-particular nature of these actions cloud attempts at highly specific, history-matching efforts. As an example, averaging potentially bi-modal or multi-modal concentration behavior will likely result in overall inventory agreement with reference values at a consolidated level of resolution for a group of sites, but will usually result in poor individual site comparisons. Because of the statistical nature used in describing the waste streams, site inventories and granularity of the data and the assumptions used in the model, a certain number of these inventory comparisons may not be within the quantified uncertainty for a series of site-analyte combinations.

Significant limitations of SIM are associated with the assumptions made regarding the presence or absence of an unquantified analyte for a non-HDW Model waste stream and the assumption

regarding the separations processes being well defined and operated within specifications. The estimation of trace analytes using "less than" values, assuming contamination and dilution levels for non-HDW Model waste streams, or assuming non-quantified analytes equal zero is an extremely speculative exercise that resists rigorous quantification. Furthermore, the batch to batch processing variability and the different degrees of effectiveness with which solids were entrained and lost to the ground or retained in the tank-canyon system can be highly specific to a site or timeframe and not be representative of the total campaign associated with an operation or disposal site when abstracted to an overall model-level assumption, thus introducing a potential source of bias

As documented in several references (Healy 1953; Ruppert and Heid 1954; Paas and Heid 1955; Abrams 1956), significant challenges existed in obtaining surveillance data, and there is often sufficient evidence to call the reference data values into question, either from the inconsistencies/discontinuities observed in the record or in the calculation of the reference value (e.g., arithmetic error, changes in bases, or refinement in judgment regarding the physical/chemical behavior of analytes in the tank-canyon environment). Some of these observed reasons include:

- Inconsistent data gathering during the early Hanford Site production era resulted in annual inventory values that may have varied by as much as two to four times the presented value;

- Changes in analytical procedures that resulted in changes in observed values by a factor of 100;

- Use of detection limit values in quantifying inventory, but no indication is given that the presented value represents an upper bound;

- The impact of colloidal particles on inventory in certain disposal sites is uncertain where the conditions for their potential presence are intermittent and unpredictable; and

- Consolidation of the waste tank-disposal site inventory into a single reported value, instead of reporting individual site inventories.

Where these particular instances impact the evaluation of a site, the disagreement with the reference value is acknowledged and the technical reasoning and references are included in an exceptions table in the SIM report. If the error is correctable, the correction is incorporated, and the site remains as part of the evaluation process; if the error or basis change does not allow for a clear evaluation of the model estimate versus the reference data, it is excluded from the evaluation. At this time, if the reference data are in conflict with currently accepted convention regarding process behavior or tank chemistry, the accepted convention represents the baseline (any exceptions to this condition are noted).

Other available process and surveillance data were used in defining and assigning waste streams that were not included in the HDW; however, the nomenclature used in the various references describing the wastes being disposed is often ambiguous with regard to waste assignment to the

disposal site with little supporting analytical data and thus open to interpretation. Misassignment of waste streams with generic designations but widely varying compositions as a function of their generation and disposal during production (e.g., a label of PUREX condensate could potentially be considered either PUREX process condensate—this waste results from the direct reduction of high-level waste and likely has significant radionuclide content; or PUREX steam condensate—this waste is the result of non-contact cooling water or process water that has little if any contamination) is a potentially significant error requiring an independent data source to provide a means of correction. These discrepancies require judgment on the part of the analyst to resolve, and in certain cases, the decision to accept one source over another may have introduced an error. Thus, there is the opportunity to introduce human error/differences in technical judgment as part of the data input process of SIM. The modelers have endeavored to minimize this area for potential discrepancy; however, with a model this large, there always exists the chance for an error or oversight to occur.

7.6 RECOMMENDED FUTURE WORK

The following is recommended future work:

- Further audit the reference values and correct inconsistent or erroneous data;
- Using the qualitative and quantitative information in the reference data, estimate uncertainties for the presented values and evaluate the SIM outputs with better statistical methods;
- Develop greater spatial resolution in modeling the contaminant inventories and volume receipts for complicated, high volume sites such as 216-U-10;
- Revise the HDW Model Rev. 5 compositions and solubilities for select waste streams to agree with observation;
- Revisit the uncertainty basis and definitions for the waste streams (chemical and radionuclide) to more closely quantify the inventory uncertainty;
- Increase the HDW and/or SIM waste stream basis set;
- Verify HDW Model compositions where possible using available historical data; and
- Evaluate annual SIM estimates against available reference data or contemporary field data for selected sites, instead of only comparing the consolidated site reference values.

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