Model Package Report: Hanford Soil Inventory
Model SIM v.2
Build 1

Prepared for the U.S. Department of Energy
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Model Package Report
Hanford Soil Inventory Model

SIM v.2
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Prepared for:
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Executive Summary

The Hanford Soil Inventory Model (SIM) is a tool for the estimation of inventory of contaminants that were released to soil from liquid discharges during the U.S. Department of Energy’s Hanford Site operations. This model package report documents the construction and development of a second version of SIM (SIM-v2) to support the needs of Hanford Site Composite Analysis.

The SIM-v2 is implemented using GoldSim Pro®\(^1\) software with a new model architecture that preserves the uncertainty in inventory estimates while reducing the computational burden (compared to the previous version) and allowing more traceability and transparency in calculation methodology. The calculation architecture is designed in such a manner that future updates to the waste stream composition along with addition or deletion of waste sites can be performed with relative ease. In addition, the new computational platform allows for continued hardware upgrade.

While the input (and output) format used in the calculations remains unchanged from the previous version, the inventory calculation methodology adopted in SIM-v2 is different and avoids sampling a large number of probability density functions using the Monte Carlo sampling based calculation approach that led to a large number of realizations for estimating uncertainty in inventory. The current implementation of SIM-v2 uses an analytic approach to calculate the inventory mean and variance. The inputs defined by PDFs of waste stream densities, concentrations, and discharged volumes are assumed to be independent random variables, consistent with the assumptions of previous version, and are therefore pair-wise independent. This direct or analytic calculation of the inventory statistics is exact and requires no sampling. The results for a record (waste site, time, and analyte) are presented as inventory mean value and standard deviation of a log normal distribution function.

The new SIM-v2 model evaluates the uncertainty in liquid discharge inventory for about 400 waste sites over a time period of 58 years (1944-2001) for 76 analytes. Approximately 200 waste stream compositions are considered.

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\(^1\) GoldSim Pro is a registered trademark of GoldSim Technologies of Issaquah, Washington.
# Contents

## 1 Purpose

1.1 Need ............................................................................................................................................... 1  
1.2 Background .................................................................................................................................. 1  
1.3 Document Organization ............................................................................................................ 2  

## 2 Model Objectives

2.1 Model Objective 1: Migrate the Hardware and Software Implementation to Modern, Maintainable Platform. .............................................................................................................. 3  
2.2 Model Objective 2: Implement Analytical Approach to Efficiently Estimate the Uncertainty of the Inventory ......................................................................................................................... 3  
2.3 Model Objective 3: Implement Model Structure to Enable Addition of New Waste Sites and Waste Stream Compositions ..................................................................................................... 4  
2.4 Model Objective 4: Implement Model in Compliance with Current Quality Assurance Requirements. ................................................................................................................................................. 4  

## 3 Model Conceptualization

3.1 SIM Concepts ............................................................................................................................ 4  
3.2 Database Design ........................................................................................................................ 5  
3.3 Distribution Statistics ................................................................................................................ 5  
3.3.1 Normal Distribution: Distribution Type = 0 .................................................................. 5  
3.3.2 Triangular Distribution: Distribution Type = 1 .............................................................. 5  
3.3.3 Lognormal Distribution: Distribution Type = 4 ............................................................. 5  
3.3.4 Exponential Distribution: Distribution Type = 6 ........................................................... 7  
3.3.5 Generalized Beta Distribution: Distribution Type = 9 ................................................... 8  
3.4 Inventory Calculation ................................................................................................................ 8  
3.4.1 Parameter Units. ........................................................................................................... 10  
3.4.2 Analytic Calculation for Mean and Variance............................................................... 10  
3.4.3 Cumulative Calculations .............................................................................................. 11  

## 4 Model Implementation

4.1 Software .................................................................................................................................. 11  
4.2 Discretization........................................................................................................................... 11  
4.3 Parameterization...................................................................................................................... 12  
4.4 Calibration............................................................................................................................... 12  
4.5 Model Structure....................................................................................................................... 12  
4.6 Looping to Evaluate Site Inventories ...................................................................................... 13  
4.7 Operable Unit Associations .................................................................................................... 14  
4.8 Model Results.......................................................................................................................... 14  
4.8.1 SIM-v2 Implementation Platform Robustness............................................................. 14  
4.8.2 Comparisons Using SIM-v1 Input ............................................................................... 15  

iv
4.8.3 Scatter Plot Comparisons of SIM-v1 and SIM-v2 Using Consistent Input data........... 17
4.8.4 Comparisons of SIM Versions Using Updated SIM-v2 Input.............................. 18
5 Model Limitations .............................................................................................................. 20
6 Model Configuration Management ...................................................................................... 20
6.1 SIM-v2 Build and Application History ........................................................................ 20
6.1.1 SIM-v2 Build 1.0 ..................................................................................................... 20
7 Model Recommendations ..................................................................................................... 20
8 References .......................................................................................................................... 21

Appendices

Appendix A: SIM-v2 Analytes ................................................................................................. 23
Appendix B: Calculations Supporting the Evaluation of the Bounded Lognormal Statistics ..... 26
Appendix C: GoldSim Script Element for Evaluation of Statistics for all Distributions .......... 29
Appendix D: Architecture of the GoldSim SIM-v2 Layered Graphical Implementation ...... 33

Figures

Figure 4-1. Statistics Sub-model for Liquid Concentrations ............................................... 13
Figure 4-2. Calculation of Liquid Inventory Mean and Variance at each Time and Site ....... 13
Figure 4-3. Inventory Output Organized by Operable Units ............................................. 14
Figure 4-4. Cumulative Distribution: Site 216-A-8, Year 1955, Analyte Pb ....................... 16
Figure 4-5. History of 5th Percentile for Site 216-A-8 and Analyte Pb ............................... 16
Figure 4-6. History of 50th Percentile for Site 216-A-8 and Analyte Pb ......................... 17
Figure 4-7. History of 95th Percentile for Site 216-A-8 and Analyte Pb ............................ 17
Figure 4-8. Comparison of SIM-v1 and SIM-v2 Estimated Cumulative Mean Activity of Radionuclides and Cumulative Mass of Chemicals Discharged to Site 200-E-100 ..... 18
Figure 4-9: Comparison of Technetium-99 updated inventory of SIM-v2 and SIM-v1 ...... 19
Figure 4-10: Comparison of Uranium-238 updated inventory of SIM-v2 and SIM-v1 ...... 19

Figure D-1. Front End of SIM-v2 Code ............................................................................... 34
Figure D-2. Liquid Density Statistics Calculation ............................................................. 35
Figure D-3. Concentration Input ....................................................................................... 36
Figure D-4. Calculation of Liquid Concentration Statistics ............................................. 37
Figure D-5. Containers for Calculation of the Volume Statistics and Active Times for Current Site (SubModel_Inventory contains the inventory calculations) ........................ 38
Figure D-6. Loop Over all Volume Records (SiteInput) (Calculation index of the first occurrence of current site records and index of last occurrence of current site records. Calculate number of site records) ............................................................................................................................. 39

Figure D-7. Calculation of Total Volume Statistics ............................................................................................................. 40
Figure D-8. Top End of the Submodel Container SubModel_Inventory ............................................................................... 41
Figure D-9. Calculates Analyte Inventory Statistics for Current Site and Current Time ............................................... 42
Figure D-10. Calculations for Liquid Inventory Mean and Variance .................................................................................. 43

Tables

Table 4-1. Comparison of SIM-v1 and SIM-v2 Inventory Statistics for Operable Unit 200-PW-3 .......... 15
Terms

BBI  Best Basis Inventory
CA   Composite Analysis
DOE  U.S. Department of Energy
EMMA Environmental Model Management Archive
HDW  Hanford Defined Waste (model)
DKPRO Code to perform separations on 46 radionuclides from ORIGEN2 output
OCB  Open Crystal Ball®
ORIGEN2 Burnup code that calculates fission and activation products
OPU  Operable Unit
SIM  Soil Inventory Model
SIM-v1 Original SIM implementation in Excel®
SIM-v2 Updated SIM implementation in GoldSim®
WMA  Waste Management Area
1 Purpose

The Hanford Soil Inventory Model (SIM) is a tool for the estimation of the probabilistic inventory of contaminants that were released to soil during the U.S. Department of Energy’s (DOE’s) Hanford Site mission from 1944 until 2001. The first SIM version (SIM-v1) was implemented using Oracle Open Crystal Ball® software and Microsoft Excel® (RPP-26744, Hanford Soil Inventory Model) and reported the discharged inventory, including uncertainty in the inventory estimate, at waste sites. This model package report documents the construction and development of a second version of SIM (SIM-v2) that is implemented in GoldSim Pro® software. Thus, the scope of this model package report is to document the analytical methodology used in SIM-v2 and to demonstrate that it produces comparable output as SIM-v1 when run using the same input. The results of the updated inventory calculations for various waste sites are documented in a separate environmental calculation file (ECF-HANFORD-17-0079) along with details regarding the updated inputs for usage in the Hanford Site Composite Analysis (CA).

The Hanford SIM (SIM-v2) estimates discharged inventories of 29 chemicals and 46 radionuclides (Appendix A) over 58 years (1944-2001) of evaluation period. Currently, the calculations are performed for about 400 waste sites using 200 waste stream compositions. However, the number of waste sites and waste streams can be varied in the model for any future expansion.

1.1 Need

Prior to development of SIM-v2, an assessment was performed on SIM-v1 configuration and maintenance. Based on that assessment, the following needs were identified.

1) The dedicated hardware platform for the SIM-v1 (acquired circa 2007) is aging and is no longer rated reliable for future SIM support;

2) The calculation engine implemented using Oracle Open Crystal Ball® software is no longer available, and the license is non-transferrable to new hardware.

3) The large number of realizations required to reach statistical stability in inventory estimates led to long run times and were deemed unnecessary. The calculation methodology could be improved.

4) The SIM-v1 has several known corrective actions that require new implementation with more efficient calculation time. The known corrective actions are input related and, therefore, required model application in (ECF-HANFORD-17-0079).

1.2 Background

The prior SIM version (SIM-v1) integrated results from the Hanford Defined Waste (HDW) Model tools (LA-UR-96-3860, Hanford Tank Chemical and Radionuclide Inventories: HDW Model Rev. 4; RPP-19822, Hanford Defined Waste Model – Revision 5.0) and extended the inventory and uncertainty estimates for 46 radionuclides and 29 chemicals using approximately 200 waste streams applied to about 400 liquid waste disposal sites, UPRs, and tank leaks (RPP-26744). The SIM-v1 results were reported from 1944 to 2001 and the inventory was estimated in one-year increments.

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2 Open Crystal Ball was a registered trademark of Decisioneering of Denver, Colorado; now a registered trademark of Oracle Corporation and/or its affiliates.

3 Excel is a registered trademark of Microsoft Corporation in the United States and other countries.

4 GoldSim Pro is a registered trademark of GoldSim Technologies of Issaquah, Washington.
SIM-v1 process knowledge quantify inventories and uncertainties of liquid waste disposal sites, UPRs 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. 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. 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 UPRs (e.g., overfilling tanks, piping breaches, and other miscellaneous infrastructure failures) or from tank farm leaks.

SIM-v1 used stochastic simulations to estimate mass balanced inventories with uncertainties for the Hanford Site. A Monte Carlo based sampling approach was used as the stochastic modeling approach to provide best estimates along with uncertainty in the discharged inventory. SIM-v1 used Microsoft Excel® with the Oracle Open Crystal Ball® (OCB) statistical package for sampling the uncertainty distributions. This prior implementation SIM-v1 was coupled with specific hardware due to the license protection for OCB, which is no longer supported. In addition, the Monte Carlo sampling approach required about 25,000 realizations to produce statistical stability at the tails of the distribution as a requirement of the sampling algorithm, e.g. Latin hypercube sampling.

In the current implementation (SIM-v2), an analytical modeling approach is developed and implemented in GoldSim to propagate uncertainty. Uncertainty is estimated analytically eliminating the need to run multiple realizations saving computational burden and time. The analytical solution was feasible because the input distributions are uncorrelated. Nevertheless, GoldSim allows Monte Carlo simulations and, therefore, allows flexibility of future expansion of the SIM with correlated inputs, e.g. updating the inventory after remediation and clean up.

1.3 Document Organization

This M is organized following the structure specified in CH2M HILL Plateau Remediation Company’s Quality Assurance Project Plan for Modeling (CHPRC-00189, Appendix G):

- In Chapter 1 (this Chapter), the main needs for the model are identified in terms of functional requirements.
- In Chapter 2, the objectives of the current upgrade of SIM-v1 to SIM-v2 are described, highlighting the importance of changing the implementation platform and filling in known data gaps.
- In Chapter 3, the analytical approach and input distributions are described. The parameters describing the distribution types are defined. The corresponding formulae of the mean and standard deviations are provided for each distribution. The analytical approach describes how input uncertainty is analytically propagated by the computational rules for the mean and variance of a sum or product of independent random variables.
- In Chapter 4, the model implementation and results are described. The site data dimensions and structures are highlighted as they guide the model implementation. The SIM-Analytic solution in GoldSim is described by highlighting the main computational architecture. Details on model architecture and scripts are given in the appendices. The results of the SIM-v2 inventory calculations are compared to the sampled results of SIM-v1 Monte Carlo approach.
- Chapters 5 and 6 are brief listings of limitations and potential improvements to the GoldSim model. Identifying data gaps will guide future updates of the inventory and will identify future modeling needs.
2 Model Objectives

The objective of prior development of SIM-v1 was to provide a probabilistic approach to estimate inventory uncertainty for the waste sites receiving primarily liquid discharges at Hanford Site. This approach was previously needed to support the System Assessment Capability, which from 2000 to 2006 was implemented to support development of an updated Hanford Site Composite Analysis and was also useful to other Hanford Site remediation projects. Development and use of the System Assessment Capability was suspended in 2006 while the Tank Closure and Waste Management Environmental Impact Statement (DOE/EIS-0391) was being prepared. During that time, the SIM-v1 and a dedicated hardware platform were maintained in standby status. The objectives for SIM-v2 is to continue to meet the original objective of SIM-v1 while overcoming the following limitations:

1. The SIM-v1 was implemented using a third-party probabilistic tool (Oracle CrystalBall) that is no longer supported, and the license is non-transferrable to new hardware;
2. The dedicated hardware platform for the SIM-v1 (acquired circa 2007) is aging and is no longer rated reliable for future SIM support;
3. The SIM-v1 has several known corrective actions that require input update and model application as part of inventory maintenance.
4. The SIM-v1 was never qualified to NQA-1, which is now required under DOE O 414.1d, Quality Assurance.

To fulfill these objectives, the current model and software implementation are designed to achieve four primary objectives identified and discussed in the subsections that follow.

2.1 Model Objective 1: Migrate the Hardware and Software Implementation to Modern, Maintainable Platform.

This model objective was prioritized because the SIM-v1 is reliant on outdated hardware and software platform, and migration to a new hardware platform is not possible without changes to the software. The new version (SIM-v2) is implemented using GoldSim® software that is compatible with modern computer hardware and operating systems. GoldSim licensing is portable, and the software supports a module to enable distributed computing – a valuable feature to efficiently run complex models or large probabilistic calculations under Monte Carlo approaches. SIM-v2 is implemented using both graphical programming and scripting techniques available in GoldSim.

2.2 Model Objective 2: Implement Analytical Approach to Efficiently Estimate the Uncertainty of the Inventory

This model objective is to improve the accuracy in propagating uncertainty, and to speed up the computation, thereby allowing for a more integrated analysis of Hanford site-wide analysis. The SIM-v1 calculation methodology based on Monte Carlo sampling approach required about 25,000 realizations to produce statistical stability at the tails of the sampled distribution of the probability density functions. This required a long computational time which SIM-v2 greatly improves upon. The inventory estimates at any percentile can be directly calculated from the analytical approach without consideration of statistical stability.
2.3 Model Objective 3: Implement Model Structure to Enable Addition of New Waste Sites and Waste Stream Compositions

Implement calculations in nested loops to allow flexibility for adding any number of waste sites and waste streams by adjusting loop counters according to input records. This also allows for updating uncertainty inputs for estimating inventory of UPRs and tank leaks as more information is now available from monitoring systems and tank leak studies.

2.4 Model Objective 4: Implement Model in Compliance with Current Quality Assurance Requirements

The SIM-v2 will support regulatory decisions at the Hanford Site, including the preparation of a revised Hanford Site Composite Analysis as well as other uses. Therefore, this model requires a stringent level of quality assurance.

GoldSim has been qualified for use as Safety Software, Level C at the Hanford Site (CHPRC-00175, CHPRC-00180, GoldSim Pro Functional Requirements Document, GoldSim Pro Software Management Plan; CHPRC-00224, GoldSim Pro Software Test Plan; CHPRC-00262, GoldSim Pro Acceptance Test Report; CHPRC-00256, GoldSim Pro Requirements Traceability Matrix). Thus, implementation of the SIM-v2 in GoldSim will meet the DOE O 414.1d requirements for controlled software use.

The quality assurance of the SIM-v2 as a model will be met through compliance with the requirements of CHPRC’s Quality Assurance Project Plan for Modeling (CHPRC-00189, Appendix E). The model follows an analytical approach to propagate and estimate uncertainty of discharged liquid inventory. The non-parametrized nature of the model and applied analytical approach does not require calibration and sensitivity analysis.

3 Model Conceptualization

This section provides the conceptual basis for the SIM-v2 mathematical model.

3.1 SIM Concepts

Contaminants in waste streams can occur as solutes and entrained solids. Parameters which determine inventory are liquid and solid waste stream densities, liquid and solid waste stream concentrations for all analytes (contaminants), and for each site the time history for the total volume and solid volume fraction of each waste stream. Uncertainty for each parameter record is described by a probability distribution. The density, concentration and volume data are compiled in a Microsoft Excel file, which for simplicity is referenced subsequently as SIM_Input.

The SIM-v1 code sampled all uncertain parameter distributions and calculated a resulting sampled inventory value for each site, time, and analyte. By performing 25,000 realizations, the inventory sampled mean was calculated along with percentiles ranging from 0.5th to 99.5th. It is emphasized that the SIM-v1 inventory statistics are sample statistics generated from the 25,000 Monte Carlo realizations.

The current implementation of SIM-v2 uses the GoldSim software to calculate the inventory statistics directly from the uncertainty distributions for density, concentration, total volume, and volume fraction solid. The inventory statistics are calculated directly from the underlying distributions that require no sampling and therefore the results are exact. The statistics for an inventory record (site, time, and analyte) calculated by the SIM-v2 model are mean and standard deviation.
3.2 Database Design

The SIM-v2 uses the same input database (SIM_Input) as the SIM-v1 model for the uncertainty parameters representing density, concentration, volume total and volume fraction solids. In addition, SIM-v2 requires information describing the sites within each Operable Unit. The input file is organized within one Excel workbook with distinct sheets for the density, concentration, volume, and Operable Unit/site data. Inventory output is also organized with an output file for each Operable Unit. Within an Operable Unit output file each site inventory results are reported to a site-specific sheet.

3.3 Distribution Statistics

The distribution types used to represent density, concentration, and volume uncertainty include normal, triangular, lognormal, truncated lognormal, exponential, and generalized beta. The SIM-v2 inventory statistics calculation methodology requires the distribution mean and variance for each input record. The distribution mean and variance calculations are discussed for each distribution type in the subsequent section. The distribution type is specified in the SIM_Input file by a distribution index number as noted below.

3.3.1 Normal Distribution: Distribution Type = 0

The normal distribution parameters are mean and standard deviation

- parameter1: $\mu = \text{mean}$
- parameter2: $\sigma = \text{standard deviation}$

The only calculation required is

$$\text{variance} \ (\text{var}) = \sigma^2.$$

3.3.2 Triangular Distribution: Distribution Type = 1

The triangular distribution has parameters

- parameter1: $a = \text{minimum}$
- parameter2: $c = \text{mode}$
- parameter3: $b = \text{maximum}$.

The triangular distribution statistics are

$$\mu = \frac{a + b + c}{3}$$

$$\text{var} = \frac{a^2 + b^2 + c^2 - ab - ac - bc}{18}.$$

3.3.3 Lognormal Distribution: Distribution Type = 4

The lognormal distribution occurs as both a two-parameter and a three-parameter distribution. The two-parameter lognormal is used to describe liquid and solid density uncertainty. The lognormal distribution parameters are
parameter 1: \( \mu = \) mean

parameter 2: \( \sigma = \) standard deviation.

Data base parameters for three-parameter truncated lognormal distribution are used to describe concentration and volume uncertainty. Database parameters are

parameter 1: \( \mu = \) mean

parameter 2: \( \sigma = \) standard deviation

parameter 3: \( b = \) upper truncation value,

where the mean and standard deviation are values for the two-parameter lognormal distribution or unbounded lognormal.

The truncated lognormal distribution depends on the following

\( X = \) random variable with lognormal distribution

\( X_b = \) random variable with truncated lognormal distribution

\( Y = \) normal distribution with \( Y = \ln(X) \)

\( \mu_X = \) Arithmetic mean of lognormal distribution

\( \sigma_X = \) Arithmetic standard deviation of lognormal distribution

\( \mu_Y = \) Expected value of \( \ln(X) \)

\( \sigma_Y = \) standard deviation of \( \ln(X) \)

\( b = \) upper bound for the truncated lognormal distribution.

Then

\[
\mu_Y = \ln(\mu_X) - \frac{1}{2} \ln \left( 1 + \frac{\sigma_X^2}{\mu_X^2} \right) = \ln \left( \frac{\mu_X^2}{\sqrt{\mu_X^2 + \sigma_X^2}} \right)
\]

\[
\sigma_Y = \sqrt{\ln \left( 1 + \frac{\sigma_X^2}{\mu_X^2} \right)} = \sqrt{\ln \left( \frac{\mu_X^2 + \sigma_X^2}{\mu_X^2} \right)}
\]

If the probability density function for the lognormal distribution \( X \) is denoted \( f(x) \), \( 0 < x < \infty \), then the probability density function for the truncated lognormal distribution \( X_b \) is

Specifying a maximum value for the variable \( X \) that is presented by the lognormal distribution changes the distribution and the values of its statistical parameters. The new parameter values can be evaluated analytically by introducing the error function (erf) and its complementary error function (erfc) listed in
Appendix B. The introduction of the erf/erfc is an analytical technique to perform the needed integral bounded by the specified maximum.

\[ f_b(x) = \frac{f(x)}{F(b)}, \quad 0 < x \leq b, \]

where \( F(x) \) is the cumulative distribution function for random variable \( X \). That \( f_b(x) \) is a probability density function follows from

\[
\int_0^b f_b(x) \, dx = \frac{1}{F(b)} \int_0^b f(x) \, dx = \frac{F(b)}{F(b)} = 1
\]

From results B1 and B2 in Appendix B, the mean of the truncated lognormal is computed by

\[
\mu_{x_b} = \frac{1}{F(b)} \left[ \mu_x - \mu_x \frac{\text{erfc} \left( -\frac{\mu_Y + \sigma_Y^2 - \ln(b)}{\sqrt{2}\sigma_Y} \right)}{2} \right]
\]

\[
= \frac{\mu_x}{2F(b)} \left[ 2 - \text{erfc} \left( -\frac{\mu_Y + \sigma_Y^2 - \ln(b)}{\sqrt{2}\sigma_Y} \right) \right] = \frac{\mu_x}{2F(b)} \text{erfc} \left( \frac{\mu_Y + \sigma_Y^2 - \ln(b)}{\sqrt{2}\sigma_Y} \right).
\]

A similar integration yields the truncated lognormal 2\textsuperscript{nd} moment

\[
E[X_b^2] = \frac{\exp \left( 2(\mu_x + \sigma_Y^2) \right)}{2F(b)} \text{erfc} \left( \frac{\mu_y + 2\sigma_Y^2 - \ln(b)}{\sqrt{2}\sigma_Y} \right)
\]

and variance

\[
\sigma_{x_b}^2 = E[X_b^2] - \mu_{x_b}^2.
\]

3.3.4 Exponential Distribution: Distribution Type = 6

Database parameter for exponential distribution is

Parameter1: \( r = \text{rate} \).

The statistics for the exponential distribution are

\[
\mu = \frac{1}{r}
\]

\[
\sigma^2 = \frac{1}{r^2}.
\]
3.3.5 Generalized Beta Distribution: Distribution Type = 9

The generalized beta distribution is used to describe some liquid and solid concentrations. The database parameters for all generalized beta distributions are:

- parameter1: $\alpha$
- parameter2: $\beta$
- parameter3: maximum
- parameter4: minimum

The mean and standard deviation of the generalized beta distribution is:

$$\mu = \min + \frac{\alpha}{\alpha + \beta} (\max - \min)$$

$$\sigma = \frac{\max - \min}{\alpha + \beta} \sqrt{\frac{\alpha \beta}{\alpha + \beta + 1}}.$$

The GoldSim code imposes an upper bound constraint on the standard deviation for a generalized beta distribution. The generalized beta distribution standard deviation is required to satisfy the upper bound test:

$$\sigma^* \leq 0.6 \sqrt{\mu^* (1 - \mu^*)}$$

where

$$\mu^* = \frac{\mu - \min}{\max - \min}, \quad \sigma^* = \frac{\sigma}{\max - \min}.$$

If the upper bound test is not satisfied the standard deviation is decreased by

$$\sigma_{\beta} = (\max - \min) 0.6 \sqrt{\mu^* (1 - \mu^*)}.$$

This constraint is imposed in SIM-v2 for the generalized beta standard deviation calculation.

3.4 Inventory Calculation

At present, a total of 213 waste streams can be considered for estimating disposed inventory to the sites. Of the 213 waste streams, 205 have a defined composition (are active) and eight are null, which can be used should additional modeling needs arise.

The SIM-v2 calculations are performed from year 1944 to 2001, spanning 58 years. A total of 75 analytes are considered (chemical and radionuclides) plus the total Uranium mass. SIM-v2 reports for 80 analytes. Four additional dummy analytes (Su-232, Su-233, Su-234, and Su-235) are added to accommodate possible future addition of other analytes. If additional analytes are included in the future, the code can accommodate these new analytes without changes to the SIM-v2 code. The only change required would be the analyte names within the output file.
The analytes can occur in solution or as entrained solids. The inventory released to a site will depend on the concentrations in both liquid and solids of each analyte and each waste stream. Consequently, the liquid and solid concentration information are contained in a matrix with dimension (number_of_analytes) by (number_of_wastestreams) or [80,213]. Both liquid and solid waste stream density input are contained in a vector with dimension (number_of_wastestreams) or [213]. The volume of liquid and solids released will depend on the site, time or year, and waste stream. The input data for volumes consist of total volume and volume fraction solid, which for given site and time is a vector with dimension (number_of_wastestreams) or [213].

SIM-v2 execution calculates inventories for all sites within a specified Operable Unit. The calculation loops over all sites within the Operable Unit. For each site the inventory calculation is organized by a calculation looping over all active times for the site.

The liquid inventory (INVL) and solid inventory (INVS) for a given site and time are calculated as

\[
INVL_{\text{site, time}} = CL * DL * VT_{\text{site, time}} * (1 - VFS_{\text{site, time}})
\]

\[
INVS_{\text{site, time}} = CS * DS * VT_{\text{site, time}} * VFS_{\text{site, time}}
\]

where,

- \(na\) : number of analytes
- \(nws\) : number of waste streams.
- \(CL[na,nws]\) : liquid concentration matrix
- \(CS[na,nws]\) : solid concentration matrix
- \(DL[nws]\) : liquid density vector
- \(DS[nws]\) : solid density vector
- \(VT_{\text{site, time}}[nws]\) : total volume vector for given site and time
- \(VFS_{\text{site, time}}[nws]\) : solid fraction of total volume vector for given site and time
- \(1 - VFS_{\text{site, time}}[nws]\) : liquid fraction of total volume vector for given site and time

The output of resulting inventory calculations is the inventory mean and standard deviation. The various percentiles can be estimated by considering the statistical results to be representative of a lognormal distribution. When large number of components having arbitrary but well-behaved distributions are multiplied they result in a lognormal distribution based on the modified central limit theorem (Fullwood, 1999).

Note that if \(VFS\) is the solid fraction of total volume, then \(1 - VFS\) is the liquid fraction of total volume. The total inventory is the sum of the liquid and solid inventory

\[
INV_{\text{site, time}} = INVL_{\text{site, time}} + INVS_{\text{site, time}}
\]

Equation 3
The second and third multiplications and subtraction in Equations 1 and 2 are entry-wise multiplication/subtraction over the waste stream vectors, while the first multiplication is a matrix-vector multiplication with result a vector over all analytes.

The sum of the liquid and solid inventory statistics is provided by Equation 3.

3.4.1 Parameter Units.

Parameter units are discussed in PNNL-16099, Hanford Soil Inventory Model (SIM) Rev. 1 Users Guide. Total volume (VT) has units of mega liters (ML). Volume fraction solid (VFS) is dimensionless. Waste stream liquid and solid density have units of gram per milliliter (g/mL). Concentration units are on a mass bases. Liquid and solid concentration for chemical analytes are micro gram per gram (µg/g). Liquid and solid concentration for the radioactive analytes were changed to (µCi/kg) compared to the original unit of micro-curies per gram (µCi/g) that was considered in the SIM-v1. Thus, the conversion factor for inventory is 1 for both chemicals and radionuclides, which are reported in kg and Ci, respectively. The reason of this unit change for the radionuclide concentrations is to eliminate the scale factor of 10^9, which was used in SIM-v1 in order to accommodate the sampling procedure. Inventory is the product of concentration, density and volume and for chemical analytes has units of kilograms:

\[
CDV : \frac{\mu g}{g} \cdot \frac{g}{mL} \cdot \frac{10^6 L}{ML} \cdot \frac{10^3 mL}{L} \cdot \frac{g}{10^6 \mu g} \cdot \frac{kg}{10^3 g} = kg.
\]

For the radioactive analytes the inventory units are

\[
CDV : \frac{\mu Ci}{kg} \cdot \frac{10^{-3} kg}{g} \cdot \frac{g}{mL} \cdot \frac{10^6 L}{ML} \cdot \frac{10^3 mL}{L} \cdot \frac{10^{-6} Ci}{\mu Ci} = Ci.
\]

The unit conversion factor for both chemicals and radioactive analytes is 1.

3.4.2 Analytic Calculation for Mean and Variance

The analytic calculation of the inventory mean value and variance is a result of the independence of the density, concentration and volume uncertainty. Two random variables \(X_1\) and \(X_2\) are independent if their joint pdf satisfies

\[
f(x_1, x_2) = f(x_1)f(x_2).
\]

The concentrations, volumes and densities are assumed to be independent random variables, and are therefore pair-wise independent. As part of SIM-v1 development, input distributions of these variables were evaluated independently from variability of different campaigns. Concentration distributions were evaluated from the ORIGEN2 (ORNL/TM-7175, A User’s Manual for the ORIGEN2 Computer Code; burnup code that calculates fission and activation products) and DKPRO (HNF-SD-WM-CSWD-082, DKPRO: A Radionuclide Decay and Reprocessing Code; a Fortran code to perform separations on 46 radionuclides from ORIGEN2 output) estimates for each individual analyte during fuel processing using variability over campaigns of 5 year intervals. Volume distributions were estimated from waste transaction records. Density distributions are evaluated for each waste stream using total mass variability of its constituents and total volume variability.

Assume \(X_1\) and \(X_2\) are independent and let \(Y = X_1 + X_2\) be the sum and \(Z = X_1X_2\) be the product of the two random variables. Introduce the notation for the means and standard deviations for the two variables.
random variables $\mu_{X_i} = \mu_i$, $\sigma_{X_i} = \sigma_i$, $i = 1, 2$. The mean values of the sum and product are the sum and product of the means, respectively,

$$\mu_Y = \mu_1 + \mu_2,$$

$$\mu_Z = \mu_1 \mu_2.$$ 

The variance of the sum is the sum of variances

$$\sigma_Y^2 = \sigma_1^2 + \sigma_2^2,$$

while the variance of the product is

$$\sigma_Z^2 = \sigma_1^2 \sigma_2^2 + \mu_1^2 \sigma_2^2 + \mu_2^2 \sigma_1^2.$$ 

For sites with solids, the liquid volume fraction is $V_{FL} = 1 - V_{FS}$. The mean of the liquid volume fraction is

$$\mu_{V_{FL}} = 1 - \mu_{V_{FS}},$$

while the liquid volume fraction variance is

$$\sigma_{V_{FL}}^2 = \sigma_{V_{FS}}^2.$$ 

With the mean and variance of the concentration, density and volume distributions and mean and variance results for sum/products of independent random variables, the mean and variance of the inventory is calculated. The resulting inventory mean value and variance are exact values for the inventory statistics, while the SIM-v1 Monte Carlo results are sample mean and variance approximations to these exact values.

### 3.4.3 Cumulative Calculations

For a given site, a cumulative over time (1944-2001) is calculated for each analyte. The analyte cumulatives are summations over time, which imply the cumulative of the mean and variance are the sum over time of the mean and variance, respectively. The cumulative calculations are implemented within the Microsoft Excel output files.

### 4 Model Implementation

#### 4.1 Software

GoldSim is a versatile simulation software system for modeling complex systems in engineering, science and business. Models are built in an intuitive visual manner (see Appendix D Figures D-1 to D-10). The GoldSim architecture allows diagnostic understanding of the calculational model, answer “what if” questions about the model, and evaluation of alternative designs.

#### 4.2 Discretization

There is no discretization required for the SIM-v2 GoldSim model. Inventories are calculated on an annual basis from years 1944-2001. This concept of inventories on a yearly basis is inherited from the
input file. The model reports yearly inventory results, but the years reported are static (1944-2001). The analytic approach for the inventory statistics requires straightforward arithmetic. There are no issues of convergence. There is no need for a spatial discretization of the site locations. If the inventory results are used as source terms for future transport calculations, the site locations must be specified with respect to the finite difference grid location used in the transport calculations.

4.3 Parameterization

All necessary parameters are specified within the input file. This includes the uncertainty distributions for volumes, concentrations, and densities. The location of sites within the existing operable units is also required and is specified within the input file. All information for calculation of the inventory statistics is provided by the input file.

4.4 Calibration

No calibration of the SIM-v2 model is required since it is an analytic calculation based on the specified inputs.

4.5 Model Structure

The SIM-v2 is implemented in GoldSim in a layered structure using the "Top-down" modeling approach of GoldSim software. SIM-v2 first calculates the liquid and solid density vectors over waste streams. GoldSim then calculates the statistics for the liquid and solid concentration matrices. The volume data and inventory calculation are organized by Operable Units. The calculations for an Operable Unit are organized by sites. Results are written to an Operable Unit level file (Excel) with sites organized by sheets. For each inventory record (site, time, and analyte) the inventory mean and standard deviation are reported.

Appendix C lists the main script elements implemented in GoldSim to calculate statistics, mean and variance, for each possible distribution type as applied to volume, density, and concentration input. Appendix D describes the architecture of the graphical implementation of SIM-v2 in GoldSim showing the different model layers.

There are six sets of statistical inputs to SIM model consisting of three inputs each for liquid and solid portions: volume transactions for each site, concentration of analytes in each discharged waste stream, and density of each waste stream. Each input record specifies the distribution type as defined in Section 3.3 and the distribution parameters. Evaluations of the mean and variance of the distributions are calculated by a statistical submodel, which is shown in Figure 4-1 for liquid concentration. This submodel is repeated six times for the corresponding data sets, but names of the constituting elements are post-scripted differently:

CL: concentration of analytes in liquid portions,
CS: concentration of analytes in solids portions,
DL: density of the liquid portion of waste streams,
DS: density of the solids portions of waste streams,
VT: total discharged volume for a given year,
VFS: solid fraction of total discharged volume for a given year.
There are two reasons for repeating the same calculation submodel. First, to differentiate the liquid from the solid calculations. Second, the site/volume, concentration and density input arrays have different dimensions. GoldSim does not allow run-time changes of array dimensions; therefore, the same calculation is repeated by applying the name post scripting.

The submodel implementation is demonstrated by taking the concentration of liquids, as an example of the six implementations (Figure 4-1). The calculation of statistics for a single record is in the script element CL_Statistics. The script is listed in Appendix C. The CL_parm elements are the input parameters describing the distribution. The script calculates the mean and variance for a single record. The mean and variance are then assigned to appropriate arrays and the unit conversion factors are applied in respective scripts CL_Mean and CL_Var.

4.6 Looping to Evaluate Site Inventories

Shown in Figure D-1, container LoopOverSites loops over all sites within the current Operable Unit. Within the loop over sites the site volume statistics are computed. The inventory calculations are done within a sub-loop over the site active times. For given site and time the inventory calculations are shown in Figure 4-2. The calculation is for the inventory liquid mean and variance. The product of density times volume is a term-wise product over waste streams. The inventory calculation is the concentration matrix times the density times volume vector.
4.7 Operable Unit Associations

Waste sites are associated with CERCLA Operable Units. When executed, the GoldSim model calculates inventories for all sites within a specified Operable Unit (OPU) / Waste Management Area (WMA). The Operable Unit/site information is input defined and describes which sites are contained within a specified operable unit. The model is run for a single Operable Unit/WMA or for multiple Operable Units. To run for a single Operable Unit, the user specifies the Operable Unit index, ID_OPU, and executes the code. Multiple Operable Units can be run with an external batch file. Each statement within the batch file assigns the Operable Unit index, ID_OPU, and executes the GoldSim code. The batch file can repeat the assignment of Operable Unit index and execution of the code for any number of Operable Units. For an Operable Unit run, output is written to an Operable Unit file with site inventory results written to a site-specific sheet. Figure 4-3 show the 28 Operable Units conditional containers for output. Within each Operable Unit container are conditional site containers for all sites within the current Operable Unit.

```
OPU_200_BC_1  OPU_200_CW_1  OPU_200_EA_1  OPU_200_CM_1  OPU_200_WA_1
OPU_200_CP_1  OPU_200_CW_3  OPU_200_CM_3  OPU_200_WA_3
OPU_200_CM_1  OPU_200_CW_5  OPU_200_CM_5  OPU_200_WA_5
OPU_200_PW_1  OPU_200_PW_3  OPU_200_PW_6
OPU_200_PU_1  OPU_300_FF_1  OPU_300_FF_2
OPU_WMA_A_AX  OPU_WMA_B_AY  OPU_WMA_C
OPU_WMA_S_A  OPU_WMA_T
OPU_WMA_X  OPU_WMA_Y
OPU_WMA_Z
```

Figure 4-3. Inventory Output Organized by Operable Units

4.8 Model Results

Inventory calculations performed using SIM-v2 (analytic based) are compared to the SIM-v1 (Monte Carlo based) results to demonstrate that the current methodology is sound and implemented correctly and achieves the modeling objectives.

4.8.1 SIM-v2 Implementation Platform Robustness

The Monte Carlo sampling approach implemented in SIM-v1 required 25,000 realizations with a corresponding large calculation time. The accuracy of the sample statistics calculation depends on the number of samples and therefore requires large number of realizations. In contrast, the calculation time for the SIM-v2 model is order of magnitude less than the time taken to complete a similar SIM-v1 model run. The statistics for a Monte Carlo SIM-v1 simulation are calculated as sampled statistic values. The SIM-v2 analytic values for mean and standard deviation are exact statistics for the inventory. The inventory uncertainty as represented by the analytic mean and standard deviation calculations in SIM-v2 is a significantly more efficient calculation than SIM-v1 sample statistics and SIM-v2 provides an exact representation of inventory statistics.
4.8.2 Comparisons Using SIM-v1 Input

In assessment of the model objective 2, the SIM-v2 inventory results are compared to the SIM-v1 results this requires using identical input for both versions. The results do not represent the entire inventory but are used to demonstrate the achievement of the modeling objectives 1 and 2 and check that the SIM-v1 results are close approximations to SIM-v2 results. The calculations for each of the four sites within operable unit 200-PW-3 are compared in Table 4-1. The maximum and average relative difference in mean and standard deviations are calculated over all times and analytes.

From Table 4-1 the maximum relative difference for the mean statistic over all four sites vary between 0.13% and 1.4%, while the maximum relative difference for the standard deviation statistic over all four sites vary between 0.44% and 2.8%. The average relative difference for the mean statistic vary between 0.02% and 0.37%, while the average relative difference for the standard deviation statistic vary between 0.1% and 0.8%.

<table>
<thead>
<tr>
<th>Site Name</th>
<th>Max relative difference of mean</th>
<th>Max relative difference of standard deviation</th>
<th>Average relative difference of mean (only non-zero values considered)</th>
<th>Average relative difference of standard deviation (only non-zero values considered)</th>
</tr>
</thead>
<tbody>
<tr>
<td>216-A-24</td>
<td>1.4E-2</td>
<td>2.8E-2</td>
<td>3.7E-3</td>
<td>7.6E-3</td>
</tr>
<tr>
<td>216-A-31</td>
<td>2.5E-3</td>
<td>7.4E-3</td>
<td>5.8E-4</td>
<td>2.0E-3</td>
</tr>
<tr>
<td>216-A-7</td>
<td>1.3E-3</td>
<td>4.4E-3</td>
<td>1.8E-4</td>
<td>1.0E-3</td>
</tr>
<tr>
<td>216-A-8</td>
<td>5.0E-3</td>
<td>1.2E-2</td>
<td>6.4E-4</td>
<td>2.3E-3</td>
</tr>
</tbody>
</table>

As noted the central tendency or mean values show very good agreement between the SIM-v1 and the SIM-v2. The difference between estimated standard deviation values was larger than the difference between the corresponding mean values. The magnitude of the differences is dependent on the sample size used in SIM-v1 calculations for a given probability density function.

A cumulative distribution comparison is made in Figure 4-4. This requires selection of a specific site (216-A-8), a specific time (1955) and a specific analyte (Lead [Pb]). Lead was selected as an example since Pb exists in almost every waste stream and will contribute to the inventory calculation. The SIM-v2 cumulative inventory is derived from the calculated mean and standard deviation for a lognormal probability distribution. The cumulative results for SIM-v1 and SIM-v2 overlay.

Another comparison considers a time history of inventory at 5%, 50%, and 95% percentiles for site 216-A-8 for analyte Pb. The respective percentile time histories are shown in Figures 4-5 through 4-7. The three percentile time histories show very good agreement.
Figure 4.4. Cumulative Distribution: Site 216-A-8, Year 1955, Analyte Pb

Figure 4-5. History of 5th Percentile for Site 216-A-8 and Analyte Pb
4.8.3 Scatter Plot Comparisons of SIM-v1 and SIM-v2 Using Consistent Input Data

Display of consistent results among the two SIM versions is established through a scatter plot of the cumulative mass (for chemical analytes) or curies (for radioactive analytes) over time for a given waste site (200-E-100). The scatter plot results in Figure 4-8 demonstrates very close correlation between the analytic SIM-v2 and SIM-v1 results.
Comparisons of SIM Versions Using Updated SIM-v2 Input

For the assessment of the model objectives 3 and 4, example results of SIM-v2 are compared with SIM-v1. Detailed assessment of the updated SIM-v2 input and resulting inventory were developed and discussed in a separate document (ECF-HANFORD-17-0079). In this section, examples of the mean inventory estimates between SIM versions are presented for technetium-99 and uranium-238 for all waste sites modeled (Figures 4-9 and 4-10). Both scatter plots show that most waste sites have the same mean inventories calculated from both SIM versions. Most of the major differences result from tank farm sources (site designations starting with “241”) due to updated tank leak inventories. Other relatively large differences result from the update of waste stream compositions associated with unplanned releases (UPRs; site designations starting with “UPR-200”). Some minor changes that are apparent (differences of 20% or less) are due to rerouting of Z area waste streams (corrections for assigned low-salt and high-salt waste stream assignments) and due to concentration dilutions applied to the “216-B” waste sites. These two examples demonstrate that the relative differences among the two versions result from changes made in the inputs and not because of implementation errors.
Figure 4-9: Comparison of Technetium-99 updated inventory of SIM-v2 and SIM-v1

Figure 4-10: Comparison of Uranium-238 updated inventory of SIM-v2 and SIM-v1
5 Model Limitations

Two GoldSim software related minor limitations are identified: (1) GoldSim does not allow run-time changes of array dimensions; (2) Output parameter specifications cannot be changed dynamically during the simulations. Therefore, addition of inputs for new sites or updating existing sites requires changes to array dimensions, looping control, conditional container control, and output reporting.

The input distributions (probability density functions) are based on limited available data. The volume uncertainty is either estimated from reported maximum and minimum or from limited recorded transactions of waste. The composition of waste streams and associated uncertainty are derived using models of historical production processes and operations knowledge. As more information becomes available the uncertainty in inventory estimates would need to be refined.

6 Model Configuration Management

SIM-v2 model files will be placed in Environmental Model Management Archive (EMMA). The GoldSim software allows versioning of the model file following which any changes will be tracked and recorded as part of the change log.

Periodic updates to the SIM inputs are planned as more information becomes available from waste site characterization efforts on the Hanford Site’s Central Plateau. Furthermore, to support the fate and transport modeling additional calculation modules may be added to the current architecture. When the architecture of the SIM-v2 is modified, a new revision of this model package report will be prepared and issued to accompany the build’s release. When SIM-v2 is applied to prepare updated results, a new or revised environmental calculation package will be prepared to document the changes in model inputs and impacted results along with evidence of checking and review to demonstrate adherence to the pertinent quality assurance requirements.

6.1 SIM-v2 Build and Application History

The current build and all prior builds, and their applications, are described in this subsection.

6.1.1 SIM-v2 Build 1.0

The first released build of the SIM-v2 is Build 1.0, documented in CP-59798 Rev. 0 (this document). This replaces the older SIM-v1 implementation (using Microsoft Excel with Oracle Open Crystal Ball for Monte Carlo sampling) with a GoldSim based implementation using analytical solutions for uncertainty quantification.

The first application of SIM-v2 Build 1.0 is documented in ECF-HANFORD-17-0079 Rev. 0, Hanford Soil Inventory Model (SIM-v2) Calculated Inventory of Direct Liquid Discharges to Soil in the Hanford Site's 200 Areas.

7 Model Recommendations

Recommendations for potential future improvement of the Hanford SIM are identified in this section for reference and consideration in future work planning. This section will be revised and updated as work on the SIM-v2 implementation and maintenance continues. Identified potential improvements are as follows:
1. An improvement would be to link the SIM-v2 with a new tank inventory model that is based on HDW model and calibrated with site data from the Best Basis Inventory (BBI) (HNF-SD-WM-TI-740, HNF-SD-WM-SP-012 Rev. 4, 2002, Tank Farm Contractor Operation and Utilization Plan and the BBI update - RPP-7625 Rev.13, 2017)). This improvement will allow continuity check of prior discharges from tank to soil (e.g. cribs) as well as better definition of input distributions of the tank leak sites. In SIM-v1, the composition of any given leak was assumed to be an average of all the waste streams that were routed through the tank prior to the leak. However, distributing the leak composition in proportion to the feed volume from each waste stream during the leak period would be more relevant to estimate the leak inventories.

2. A possible improvement would be to add the capability to model inventory removal for waste sites where contaminated soils have been removed as part of the remediation process. This could be incorporated as an additional module in the GoldSim implementation.

8 References


Appendix A

SIM-v2 Analytes
Table A.1 SIM-v2 Analyte List

<table>
<thead>
<tr>
<th>ID</th>
<th>SIM-v2 analytes</th>
<th>Symbol</th>
<th>SIM-v1</th>
</tr>
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<tbody>
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<td>1</td>
<td>Sodium</td>
<td>Na</td>
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</tr>
<tr>
<td>2</td>
<td>Aluminum</td>
<td>Al</td>
<td>X</td>
</tr>
<tr>
<td>3</td>
<td>Iron</td>
<td>Fe</td>
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<tr>
<td>4</td>
<td>Chromium</td>
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<tr>
<td>5</td>
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Appendix B

Calculations Supporting the Evaluation of the Bounded Lognormal Statistics
The error function,
\[ erf(x) = \frac{2}{\sqrt{\pi}} \int_{0}^{x} e^{-t^2} \, dt , \]
satisfies the identity
\[ erf(-x) = -erf(x) . \]

The complementary error function
\[ erfc(x) = 1 - erf(x) \]
satisfies
\[ erfc(x) = \frac{2}{\sqrt{\pi}} \int_{x}^{\infty} e^{-t^2} \, dt . \]

Thus
\[ 2 - erfc(-x) = 2 - (1 - erf(-x)) = 1 + erf(-x) = 1 - erf(x) = erfc(x) \] ……………..B1

Consider the integration as required in the calculation for the truncated lognormal mean
\[ \int_{b}^{\infty} xf(x) \, dx = \frac{1}{\sigma \sqrt{2\pi}} \int_{b}^{\infty} \exp\left(-\frac{(\ln x - \mu_y)^2}{2\sigma_y^2}\right) \, dx . \]

Introduce the change of variables \( y = \ln x \) or \( x = \exp(y) . \) Then
\[ \int_{b}^{\infty} xf(x) \, dx = \frac{1}{\sigma \sqrt{2\pi}} \int_{\ln(b)}^{\infty} \exp\left(-\frac{(y - \mu_y)^2}{2\sigma_y^2}\right)e^y \, dy \]
\[ = \frac{1}{\sigma \sqrt{2\pi}} \int_{\ln(b)}^{\infty} \exp\left(-\frac{(y - (\mu_y + \sigma_y^2))^2}{2\sigma_y^2}\right) \exp\left(\mu_y + \frac{\sigma_y^2}{2}\right) \, dy \]
\[ = \frac{\mu_x}{\sigma \sqrt{2\pi}} \int_{\ln(b)}^{\infty} \exp\left(-\frac{(y - (\mu_y + \sigma_y^2))^2}{2\sigma_y^2}\right) \, dy \]

Make the substitution in the integration variable
\[ t = \frac{y - (\mu_y + \sigma_y^2)}{\sigma_y \sqrt{2}} \] and \( dy = \sigma_y \sqrt{2} \, dt . \]

Then
\[
\int_{b}^{\infty} xf(x)dx = \frac{\mu_X}{\sqrt{\pi}} \int_{c}^{\infty} e^{-t^2} dt, \quad c = \frac{\ln(b) - (\mu_Y + \sigma_Y)^2}{\sigma_Y \sqrt{2}}
\]

and

\[
\int_{b}^{\infty} xf(x)dx = \frac{\mu_X}{2} \text{erfc}\left(-\frac{\mu_Y + \sigma_Y^2 - \ln(b)}{\sigma_Y \sqrt{2}}\right)
\]
Appendix C

GoldSim Script Element for Evaluation of Statistics for all Distributions
Script Code

---------

Created: Aug 22, 2016 14:55:39
Element: VT_Statistics
Global Variables:

---------

// Implicit variable defining the result of the script.
VALUE Result

Script:

---------

VALUE Mean (variable exposed) = 0.0
VALUE Var (variable exposed) = 0.0
IF (VT_dist_type = 17) THEN
// null distribution
Mean = 0.0
Var = 0.0
END IF // 'VT_dist_type = 17'
IF (VT_dist_type=0) THEN
// normal distribution
Mean = VT_parm1
Var = VT_parm2^2
END IF // 'VT_dist_type=0'
// triangular distribution
IF (VT_dist_type=1) THEN
Mean = (VT_parm1 + VT_parm2 + VT_parm3)/3
Var = (VT_parm1^2 + VT_parm2^2 + VT_parm3^2 - VT_parm1*VT_parm2 - 
VT_parm1*VT_parm3 - VT_parm2*VT_parm3)/18
END IF // 'VT_dist_type=1'
IF (VT_dist_type=4) THEN
IF (VT_parm3=0) THEN
// two parameter lognormal distribution
Mean = VT_parm1
Var = VT_parm2^2
ELSE
// three parameter lognormal distribution
// mean of corresponding normal distribution
VALUE Mean_Y = 0.0
// standard deviation of corresponding normal distribution
VALUE SD_Y = 0.0
VALUE arg1 = 0.0
VALUE arg2 = 0.0
VALUE erfc1 (variable exposed) = 0
VALUE erfc2 = 0.0
VALUE FB = 0.0
Mean_Y = ln(VT_parm1) - 0.5*ln(1 + VT_parm2^2/VT_parm1^2)
SD_Y = sqrt(ln(1 + VT_parm2^2/VT_parm1^2))
arg1 = (~Mean_Y + ~SD_Y^2 - ln(VT_parm3))/sqrt(2)/~SD_Y
arg2 = (~Mean_Y + 2*~SD_Y^2 - ln(VT_parm3))/sqrt(2)/~SD_Y
erfc1 = 1 - erf(~arg1)
erfc2 = 1 - erf(~arg2)
FB = normprob((ln(VT_parm3) - ~Mean_Y)/~SD_Y)
Mean = (VT_parm1/2/~FB)*~erfc1
Var = (exp(2*(~Mean_Y + ~SD_Y^2))/2/~FB)*~erfc2 - ~Mean^2
END IF // 'VT_parm3=0'
END IF // 'VT_dist_type=4'
IF (VT_dist_type=6) THEN
// exponential distribution
Mean = 1/VT_parm1
Var = 1/VT_parm1^2
END IF // 'VT_dist_type=6'
// generalized beta distribution
IF (VT_dist_type=9) THEN
VALUE SD = 0.0
VALUE SD1 = 0.0
VALUE sd_s = 0.0
VALUE mean_s = 0.0
VALUE sd_ck = 0.0
Mean = VT_parm4 + (VT_parm3 - VT_parm4)*VT_parm1/(VT_parm1 + VT_parm2)
SD = ((VT_parm3 - VT_parm4)/(VT_parm1 + VT_parm2))*sqrt(VT_parm1*VT_parm2/(1 + VT_parm1 + VT_parm2))
// standard deviation check
mean_s = (~Mean - VT_parm4)/(VT_parm3 - VT_parm4)
sd_s = ~SD/(VT_parm3 - VT_parm4)
sd_ck = 0.5999*sqrt(~mean_s*(1 - ~mean_s))
IF (~sd_s <= ~sd_ck) THEN
Var = ~SD*~SD
ELSE
SD1 = (VT_parm3 - VT_parm4)*~sd_ck
Var = ~SD1*~SD1
END IF // '~sd_s <= ~sd_ck'
END IF // 'VT_dist_type=9'
Appendix D

Architecture of the GoldSim SIM-v2 Layered Graphical Implementation
Figure D-1: Shows the front end or top level of the GoldSim code SIM-v2. The structure is organized by the inventory calculation for all sites within a specified Operable Unit. The text box describes the elements within Figure D-1. The data element ID_OPU is the Operable Unit index. Container Select_Sites reads from input the site indices specific to the Operable Unit and calculates the number of sites. The number of sites controls the looping in container LoopOverSites. The spreadsheet element Volume_Data reads all the SiteInput or volume input records.
Figure D-2: Density input is read in spreadsheet element Density\DensityData. The liquid density statistics calculations in container Density\Density_Statistics\D_Liquid are shown in Figure D-2. The distribution type and parameters have been read from the input file. The liquid density mean and variance are saved in waste stream arrays DL_Mean and DL_Var. A similar calculation for the solid density statistics is performed in container Density\Density_Statistics\D_Solid.
Figure D-3: In Concentration\Wastestream\Loop\ the spreadsheet element ConcentrationData reads the AnalyteInput data and spreadsheet element concentration_units reads the unit conversion factors for the chemical and radioactive analytes. The liquid concentration statistic arrays are calculated in container C_Liquid and solid concentration statistics arrays are calculated in container C_Solid. The data element corrfactors provides the unit conversion factors which are applied to the concentration statistics.
Figure D-4: shows the liquid concentration statistics calculation in container \Concentration\Wastestream_Loop\Analyte_Loop\C_Liquid. The liquid concentration statistics for a given record are calculated from the distribution type and input parameters in script CL_Statistics and assigned to the arrays CL_Mean and CL_Var with dimension number of analytes by number of waste streams. An analogous calculation for the solid concentration is provided in container \Concentration\Wastestream_Loop\Analyte_Loop\C_Solid.

Figure D-4. Calculation of Liquid Concentration Statistics
Figure D-5: In container `\LoopOverSites` the container `Site_Volume` contains the calculations for volume statistics for the current site and `Active_Times` calculates the active times for current site. Appropriate information is passed to `SubModel_Inventory` for the inventory calculations.

Figure D-5. Containers for Calculation of the Volume Statistics and Active Times for Current Site
(SubModel_Inventory contains the inventory calculations)
Figure D-6: In \LoopOverSites\Site_Volume\Site_Record_Indices for the current site calculate the first volume record index, Site_Record_Min_Index, and the last volume record index, Site_Record_Max_Index. The number of volume records for the current site is calculated in Number_of_Site_Records.
Figure D-7: In \LoopOverSites\Site_Volume\Site_Records_Loop\Volume_Total the total volume statistics are computed. The script VT_Statistics calculates the mean and variance for the current volume record and distribution type. The mean and variance are assigned to arrays VT_Mean and VT_Var, respectively, with array dimensions equal to the number of production history times the number of waste streams. A similar calculation for the VFS is done in container Volume_Fraction_Solid. The total volume mean and variance arrays are initialized to zero for each new site occurrence.

![Diagram showing the calculation process](image)

**Figure D-7. Calculation of Total Volume Statistics**
Figure D-8: Figure D-8 shows the top level of the submodel container SubModel_Inventory. The vector arrays Site_ID_Vector and Analyte_ID contain the current site index and a sequential indexing of the analytes; respectively. These arrays are for output purpose only. Time_Array is an array of the years of operation of the Hanford site (1944-2001). Container Time_Loop loops over all active times for the current site and computes the site inventory and reports results to an Operable Unit output file.
Figure D-9: The inventory mean and variance calculations for the current site and current active time. These values are assigned to script elements Inventory_Mean and Inventory_Var. These arrays have dimension number of analytes. The inventory statistics are written to an output file in container OPU_OutPut. The output file is identified by the Operable Unit name. The inventory statistics are written to a sheet identified by the site name.
Figure D-10: The liquid inventory is the product of the concentration multiplied by the product of liquid density and liquid volume. The propagation of the mean and variance through these calculations result in the inventory mean and variance.