Development of Soil Inventory Model (SIM) for the Hanford Site using GoldSim

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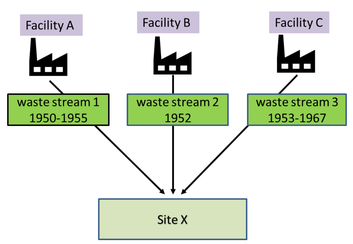
Abstract

The Hanford Site located in southeast Washington state received large volumes of liquid discharges (several billion liters) to over 400 waste sites during nuclear weapons material production mission (1944 – 1988). Over 200 types of waste streams have been identified resulting in over 6,000 records of releases to the soil. The discharged inventory of 75 constituents both chemical and radioactive is based on probability distribution functions of waste stream concentration, liquid volume released over time, and waste stream density. An analytic calculation approach is adopted, which evaluates the inventory statistical mean and variance. This description of the inventory statistics describes the uncertainty in the discharged inventory that forms the input to the contaminant transport model. The analytic calculation method is deemed superior to the Monte-Carlo sampling-based inventory calculation approach.

Purpose is to quantify uncertainty in inventory of analytes from past discharges at each of the ~400 waste sites evaluated

Introduction

Waste streams convey contaminants from facilities to sites over time



Stochastic variables which determine inventory release to a site

$$nw = number\ of\ waste\ streams$$

$$na = number\ of\ analytes$$

- Waste stream density vector: D_{nw}
- Concentration matrix: $C_{na \times nw}$
- Volume release vector: $V_{nw}(site, time)$

Inventory for a given site and time is calculated as:

$$C_{na \times nw} * (D_{nw} * V_{nw}).$$

- An early soil inventory model was developed using Monte Carlo simulation. For multiple realizations (samples) the inventory sample mean, standard deviation and cumulative distribution are computed.
- For a specified cumulative distribution criterion, the required number of samples was 25,000 (to meet convergence at tails).
- Monte Carlo calculations required an exorbitant run time and sample statistics are approximate.
- The GoldSim Analytic calculation requires approximately 2 hours for all 400 sites and statistics are exact.

SIM Analytic Approach

Basis for inventory statistics calculation

X_1 and X_2 are independent random variables and

$$Y = X_1 + X_2 \qquad Z = X_1 * X_2$$

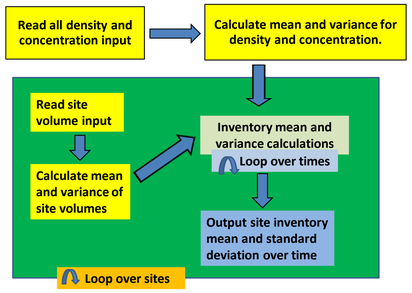
then

$$\mu_Y = \mu_1 + \mu_2 \qquad \sigma_Y^2 = \sigma_1^2 + \sigma_2^2$$

$$\mu_Z = \mu_1 \mu_2 \qquad \sigma_Z^2 = \sigma_1^2 \sigma_2^2 + \mu_1^2 \sigma_2^2 + \mu_2^2 \sigma_1^2$$

The above results for statistics of the sum and product of random variables are applied to calculate the inventory statistics.

Soil Inventory Model (SIM) Calculation Approach



Uncertainty in Waste Concentration, Volume, and Density

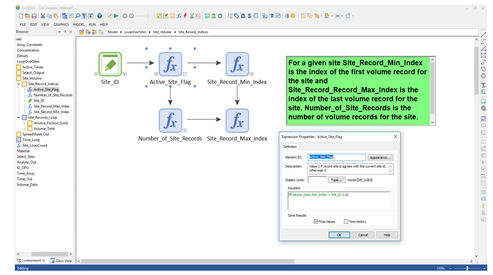
- Waste stream composition and discharge history at each waste site is compiled from literature and parameters for probability distributions are assigned in Excel input file. GoldSim reads this information from the Excel input file.
- Volume data requires the most detail and is considered in the following.
- Volume data is organized by site, time and waste stream:

Site	Waste Stream	Site Name	Year	Waste Stream Name	Distribution Type	Param 1	Param 2	Param 3	Param 4
158	18	216-B-8	1948	2C1 (BT1)	1 [=Triangular]	4.7475	6.33	7.9125	0
158	18	216-B-8	1949	2C1 (BT1)	1	5.0775	6.77	8.4625	0
158	18	216-B-8	1950	2C1 (BT1)	1	5.10975	6.813	8.51625	0
158	19	216-B-8	1950	2C2 (BT2)	1	1.485	1.98	2.475	0
158	19	216-B-8	1951	2C2 (BT2)	1	1.3725	1.83	2.2875	0
158	21	216-B-8	1951	5-6 (BT2)	1	3.87525	5.167	6.45875	0
158	21	216-B-8	1952	5-6 (BT2)	1	3.315	4.42	5.525	0
158	21	216-B-8	1953	5-6 (BT2)	1	1.46925	1.959	2.44875	0

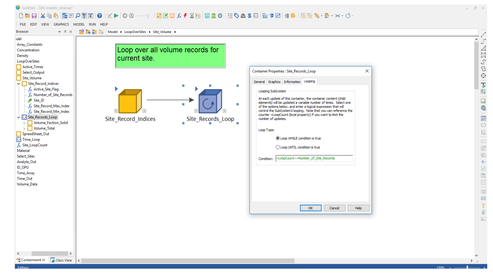
- **Script elements** are used to build arrays (vector or matrix) from calculation of a single scalar element. Also, scripts are used to build a matrix array from single vector calculations.
- VT_Statistics **script element** computes the volume mean and volume variance for a given waste site for the active time & waste stream.
- VT_Mean script element loads the mean volume result into an appropriate [time × waste stream] matrix.
- When statistics calculations for density, concentration and volume are completed for a given site, the inventory statistics calculation is performed.
- Output is organized by Site\Time\Analyte
- Inside the time loop the inventory statistics results for the site and for a single time are loaded into an array over all time

SIM Implementation

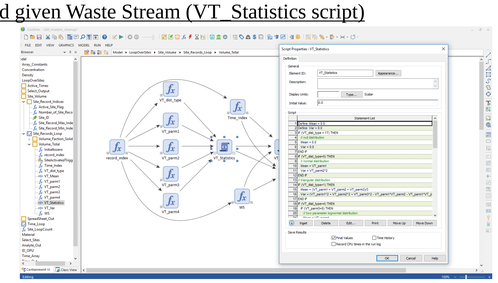
Waste Site Volume Input



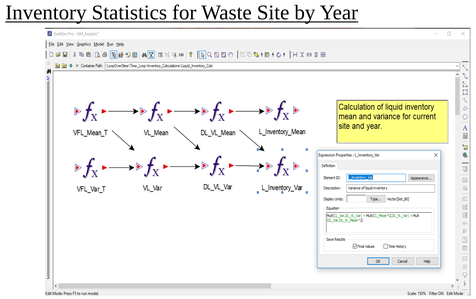
Looping to Calculate Volume Statistics for Each Waste Site



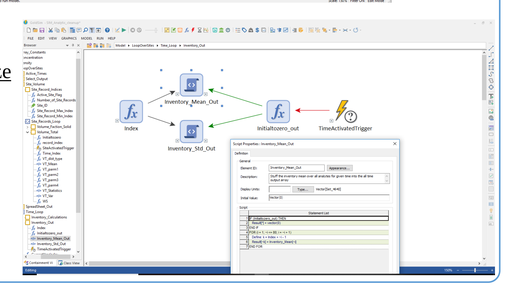
Volume Mean and Variance for a Waste Site at a given Time and given Waste Stream (VT_Statistics script)



Inventory Statistics for Waste Site by Year

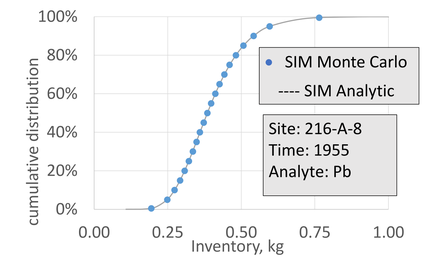


Organize Output

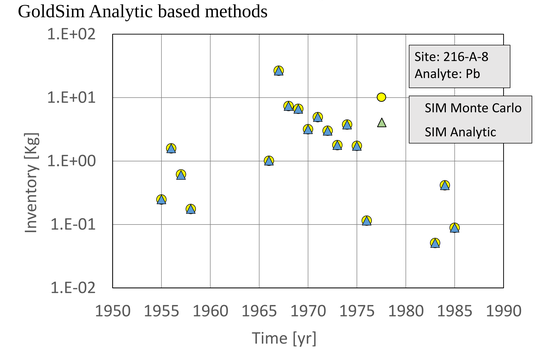


Results

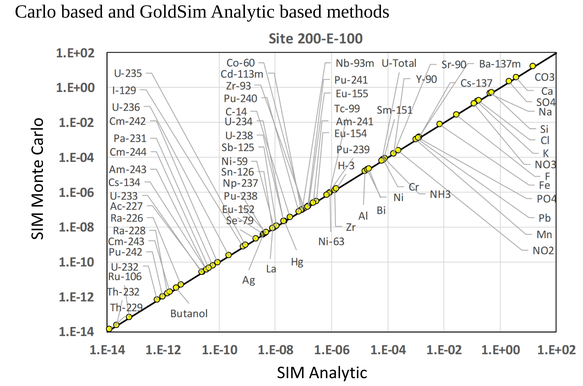
Comparison of inventory cumulative distribution between Monte Carlo based and GoldSim Analytic based method



Comparison of 5th percentile of Inventory between Monte Carlo based and GoldSim Analytic based methods



Scatter plot for all analytes comparing mean inventory between Monte Carlo based and GoldSim Analytic based methods



Summary

An analytic Soil Inventory Model (SIM) is implemented using GoldSim. The available tools in GoldSim were sufficient for reading a voluminous input file, calculation of statistics for the stochastic input variables, determination of inventory statistics, and for organizing the output.

Features such as looping containers and scripts were used extensively. The implemented analytical calculation approach is deemed superior to the previously used Monte-Carlo based sampling approach, which required 25,000 realizations.