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# Atmospheric Release Model for the E-Area Low-Level Waste Facility: Updates and Modifications

J. L. Wohlwend

November 2017

SRNL-STI-2017-00592, Revision 0

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## REVIEWS AND APPROVALS

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## **ACKNOWLEDGEMENTS**

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## EXECUTIVE SUMMARY

The atmospheric release model (ARM) utilizes GoldSim® Monte Carlo simulation software (GTG, 2017) to evaluate the flux of gaseous radionuclides as they volatilize from E-Area disposal facility waste zones, diffuse into the air-filled soil pores surrounding the waste, and emanate at the land surface. A schematic of the air pathway performance assessment (PA) analysis, after Dixon (2017), is shown in Figure E-1. The ARM is a PA model that will be treated as an “Engineering Calculation” and will not be used routinely, therefore it does not require a Software Quality Assurance Plan (SQAP). Each time results are created using ARM, the model will be design checked. This report documents the updates and modifications to the ARM for the next planned E-Area PA considering recommendations from the 2015 PA strategic planning team outlined by Butcher and Phifer (2016):

### 3.3 Non-Groundwater Pathways Calculation Improvements for Next PA Revision -RADON

- Recommendation 75
  - Load inventory and start 1,000-year assessment period at end of E-Area LLWF Operations (beginning of IC).
- Recommendation 79
  - The radionuclide screening approach used in 2008 PA was based on decay chain and half-life considerations only. For the PA revision perform radionuclide screening based on decay chain considerations only and do not include half-life in the consideration for chains leading to Rn-222 (i.e., screen full decay chains). However, screen out Rn-220 from consideration based on its very short half-life.

### 3.3 Non-Groundwater Pathways Calculation Improvements for Next PA Revision -ATMOSPHERIC

- Recommendation 81
  - Update the GoldSim Atmospheric Release Model (ARM) for vapor-phase transport to land surface.
  - Incorporate new DRF’s, latest estimated material properties and any new modeling timeline considerations.
  - Account for H3\_IP2 and H3\_TPB waste forms disposed in ILV.
  - Prepare software QA documentation for updated model.
- Recommendation 83
  - Load inventory and start 1,000-year assessment period at end of E-Area LLWF Operations (beginning of IC).
    - During IC period – Site boundary POA
    - Following IC – 100-m facility boundary POA

### 3.4.2 Use of Existing 2008 E-Area LLWF PA Models and Results

- Recommendation 38
  - For Air Pathway analysis utilize existing 1-D GoldSim ARM model, update with new data.

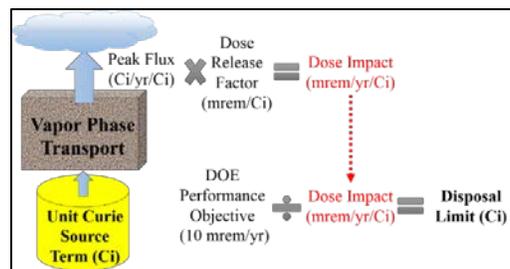


Figure E-1. Air Pathway PA Schematic

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## LIST OF ABBREVIATIONS

ARM	Atmospheric Release Model
CB/TS	Core Barrel / Thermal Shield
CCB	Controlled Compacted Backfill
CIG	Components in Grout
CLSM	Consolidated Low Strength Material
DRF	Dose Release Factor
EB	Erosion Barrier
ET	Engineered Trench
hr	hour
IC	Institutional Control
ILV	Intermediate Level Vault
KAPL	Knolls Atomic Power Laboratory
LAWV	Low Activity Waste Vault
LCCB	Lower Controlled Compacted Backfill
LLWF	Low-Level Waste Facility
LWZ	Lower Waste Zone
min	minute
NRCDA	Naval Reactor Component Disposal Area
OSC	Operational Soil Cover
PA	Performance Assessment
POA	Point of Assessment
SA	Special Analysis
SQAP	Software Quality Assurance Plan
SRNL	Savannah River National Laboratory
SRS	Savannah River Site
ST	Slit Trench
UVZ	Upper Vadose Zone
UWZ	Upper Waste Zone
yr	year

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## 1.0 Introduction

The 2011 SA (Special Analysis) ARM (Hiergesell, 2011), a GoldSim® model that calculates the air pathways limits for E-Area LLWF was updated using a revised modeling timeline and approved radionuclide data, material property values, and dose-release factors. In the process of performing the updates, a number of other improvements were made to the model. The updates and modifications are addressed in this report.

## 2.0 Model Updates

### 2.1 Dose Release Factors

Dose release factors (DRFs) have been updated with those given by Dixon (2017), including revised values for C-14 and H-3 as well as new DRFs for the additional radionuclides (Ar-37, Ar-39, Ar-42, Hg-194, Kr-81, Kr-85, and Xe-127) discussed in the updated air and radon pathways screening methodology by Dyer (2017). Table 2-1 lists the current recommended DRFs (mrem/Ci).

**Table 2-1. Previous (2006) and Current Dose Release Factors (mrem/Ci)**

Nuclide	Lee 2006		Dixon et al 2017	
	100 m Boundary DRF	SRS Boundary DRF	100 m Boundary DRF	SRS Boundary DRF
C-14	3.5E-01	1.1E-04	6.9E+00	2.2E-03
H-3	7.3E-03	2.2E-06	1.6E-02	4.8E-06
Ar-37	NA	NA	4.3E-07	1.4E-10
Ar-39	NA	NA	8.0E-05	2.6E-08
Ar-42	NA	NA	8.8E-05	2.8E-08
Hg-194	NA	NA	8.4E+00	2.0E-03
Hg-203	NA	NA	1.5E+00	3.5E-04
Kr-81	NA	NA	2.7E-05	8.5E-09
Kr-85	NA	NA	1.7E-04	5.4E-08
Xe-127	NA	NA	7.9E-03	2.5E-06

### 2.2 Material Properties

Additional radionuclides (Ar-37, Ar-39, Ar-42, Hg-194, Hg-203, Kr-81, Kr-85, and Xe-127) discussed in the 2017 Air Pathway Screening Methodology (Dyer, 2017) were added to the “Species” element in the GoldSim® model. Radionuclide atomic weights and half-lives were updated to comply with International Commission on Radiological Protection Publication 107 Radionuclide Data found in SRNL Radionuclide, Element and Dose Parameters Data Package\_12-30-15\_version1.1.xlsm. Table 2-2 displays the current species data where radionuclides that can exist as a volatile compound in the disposal environment are shown with the molecular formula in parentheses.

**Table 2-2. Updated Species List**

Species	Atomic Weight (g/mol)	Half-life
Ar39	38.9643	2.6900E+02 yr
C14 ( <sup>14</sup> CO <sub>2</sub> )	46.0012	5.7000E+03 yr
Cl36 (H <sup>36</sup> Cl)	36.9683	3.0100E+05 yr
H3 ( <sup>3</sup> H <sub>2</sub> O)	20.015	1.2320E+01 yr
I129 (H <sup>129</sup> I)	129.905	1.5700E+07 yr
Kr85	84.9125	1.0756E+01 yr
Pa234m	234.043	1.1700E+00 min
Pu238	238.05	8.7700E+01 yr
Ra226 ( <sup>226</sup> RaCl <sub>2</sub> )	296.931	1.6000E+03 yr
Rn222	222.018	3.8235E+00 day
S35 ( <sup>35</sup> SO <sub>2</sub> )	66.967	8.7510E+01 day
Sb124 ( <sup>124</sup> SbCl <sub>3</sub> )	230.265	6.0200E+01 day
Sb125 ( <sup>124</sup> SbCl <sub>3</sub> )	231.264	2.7586E+00 yr
Se75 (H <sub>2</sub> <sup>75</sup> Se)	76.9225	1.1978E+02 day
Se79 (H <sub>2</sub> <sup>75</sup> Se)	80.9185	2.9500E+05 yr
Sn113 ( <sup>113</sup> SnCl <sub>4</sub> )	254.717	1.1509E+02 day
Sn119m ( <sup>113</sup> SnCl <sub>4</sub> )	260.715	2.9310E+02 day
Sn121 ( <sup>113</sup> SnCl <sub>4</sub> )	262.716	2.7030E+01 hr
Sn121m ( <sup>113</sup> SnCl <sub>4</sub> )	262.716	4.3900E+01 yr
Sn123 ( <sup>113</sup> SnCl <sub>4</sub> )	264.718	1.2920E+02 day
Sn126 ( <sup>113</sup> SnCl <sub>4</sub> )	267.72	2.3000E+05 yr
Tc99 ( <sup>99</sup> TcO <sub>3</sub> )	146.903	2.1110E+05 yr
Th230	230.033	7.5380E+04 yr
Th234	234.044	2.4100E+01 day
U234	234.041	2.4550E+05 yr
U238	238.051	4.4680E+09 yr
Np234	234.043	4.4 day
Cm242	242.059	1.6280E+02 day
Cf246	246.069	3.5700E+01 hr
Pa230	230.035	1.7400E+01 day
Np238	238.051	2.1170E+00 day
Am242	242.06	1.6020E+01 hr
Am242m	242.06	1.4100E+02 yr
Ar37	36.9668	3.5040E+01 day
Ar42	41.963	3.2900E+01 yr
Kr81	80.9166	2.2900E+05 yr
Hg194	193.965	4.4000E+02 yr
Hg203	202.973	4.6612E+01 day
Xe127	126.905	3.6400E+01 day

### 3.0 Modifications

#### 3.1 Result Data Element

A spreadsheet element (“Results\_All”) was created in GoldSim® to manage the results for all containers. This element exports peak doses and fluxes, paired with their respective peak times, into the Microsoft Excel worksheets “Dose\_Limits” and Peak\_Release,” respectively. In addition, for Radon analysis, the Rn-222 peak is recorded in worksheet “Radon” along with the time of peak. The Rn-222 flux is also given at each time-step for each disposal unit in the worksheet, “Radon\_charts.”

#### 3.2 Timeline

A data element, “Start\_Time,” was created to set the timing for when the radionuclides are placed into the waste cells. This is currently set to zero, which corresponds in calendar notation to a simulation start time of 09/28/2040, based on the currently estimated end of E-Area LLWF disposal operations in FY40 (Sink 2016a).

#### 3.3 Solubility

Development of the ARM included the imposition of a constant concentration for  $^{14}\text{CO}_2$  in the vapor-filled pore spaces of cementitious materials. The basis for this is documented by Kaplan (2005) where the thermodynamic equations describing the equilibration of a C-14 waste source with high-pH water were evaluated. The study concluded that C-14 concentrations in the gaseous state will not exceed  $1.9\text{E}-07 \text{ Ci/m}^3$  (Hiergesell, 2011). A “Solubility\_Limit” data element was created to either account for C-14 solubility limits in cementitious mediums (with a value of 1), or not account for C-14 solubility limits (with a value of 0). This data element is exercised by the switch “Solubility\_Switch” which changes C-14 solubility within the data element “Solubilities” residing in the CIG and ILV waste column and the LAWV concrete roof.

#### 3.4 Saturation

Graham’s Law is utilized to describe diffusion through air where the effective diffusion coefficient,  $D_e$ , is given as the effective diffusion coefficient for Rn-222 times the square-root of the molecular weight ratio between Rn-222 and the radionuclide of interest,  $s$ :

$$D_e = D_e^{\text{Rn-222}} \sqrt{\frac{MW_{\text{Rn-222}}}{MW_s}} \quad (1)$$

Two equations are provided to calculate  $D_e^{\text{Rn-222}}$ . The first is given by Equation 2 (Rogers and Nielson, 1991):

$$D = D_o A_o n_a^{b_o}, \quad (2)$$

where

- $D_o$  is the diffusion coefficient for Rn-222 in air ( $\text{m}^2\text{s}^{-1}$ ),
- $A_o, b_o$  are empirical functions of porosity or constants (0.74 and 2.2, respectively),
- $n_a$  is air-filled porosity  $=n(1 - S)$ , and
- $S$  is volume fraction of water saturation.

The second equation is an updated diffusion correlation that is founded on a larger database (Equation 9 in Rogers and Nielson, 1991):

$$D_c = D_o n * \exp(-6Sn - 6S^{14n}). \quad (3)$$

The porosity,  $n$ , included in Equation 3 is total porosity as opposed to the air-filled porosity used in Equation 2. Because Equation 3 is based upon a larger database, it was chosen for preparation of the upcoming E-Area PA. Equation 2 is also available for use within ARM by modifying a selector if desired.

As detailed by Flach (2016), the one-dimensional form of Fick's law defining diffusive flux,  $j$ , is:

$$j = -D_i \frac{\partial c}{\partial x} \quad (4)$$

where, in a saturated media,

$$D_i \equiv nS\tau D_m \quad (5)$$

and  $D_m$  is the molecular diffusion coefficient and  $\tau$  is the tortuosity. This leads to

$$J = AnS\tau D_m \frac{\Delta c}{L} \quad (6)$$

where  $A$  is the cross-sectional area ( $m^2$ ) of the diffusive mass flux link and  $L$  is the diffusive length ( $m$ ).

In GoldSim®, the diffusive flux from cell  $i$  to cell  $j$  is given as:

$$f_{s,i \rightarrow j} = D_s \left( c_{ias} - \frac{c_{jws}}{K_{was}} \right) \quad (7)$$

where

$$D_s = \frac{A}{\frac{L_i}{d_{as}\tau_i n_i} + \frac{L_j}{d_{ws}\tau_j n_j}} \quad (8)$$

and

- $f_{s,i \rightarrow j}$  is the flux of species,  $s$ , from cell  $i$  to cell  $j$  (M/time),
- $D_s$  is the diffusive conductance for species  $s$  (i.e., C-14) in the mass flux link ( $L^3/\text{time}$ ),
- $c_{ias}$  is the dissolved concentration of species  $s$  in medium  $a$  (Air) within Cell  $i$  ( $M/L^3$ ),
- $c_{jws}$  is the dissolved concentration of species  $s$  in medium  $w$  (Water) within Cell  $j$  ( $M/L^3$ ),
- $K_{was}$  is the partition coefficient (unitless Henry's Law constant for diffusion through air) between fluid medium  $w$  (Water, in Cell  $j$ ) and fluid medium  $a$  (Air, in Cell  $i$ ) for species  $s$  ( $\text{mole/L Air/mole/L water}$ ),
- $A$  is the area of the diffusive mass flux link ( $L^2$ ),
- $L_i$  is the diffusive length for the diffusive mass flux link in Cell  $i$  ( $L$ ),
- $L_j$  is the diffusive length for the diffusive mass flux link in Cell  $j$  ( $L$ ),
- $d_{ws}$  is the diffusivity for species  $s$  for fluid  $w$  (Water, in Cell  $i$ ) ( $L^2/\text{time}$ ),
- $d_{as}$  is the diffusivity for species  $s$  for fluid  $a$  (Air, in Cell  $j$ ) ( $L^2/\text{time}$ ),

- $n_i$  is the porosity for the porous medium defined for the diffusive mass flux link in Cell  $i$ ,
- $n_j$  is the porosity for the porous medium defined for the diffusive mass flux link in Cell  $j$ ,
- $\tau_i$  is the tortuosity for the porous medium defined for the diffusive mass flux link in Cell  $i$ ,
- $\tau_j$  is the tortuosity for the porous medium defined for the diffusive mass flux link in Cell  $j$ .

To account for saturation within GoldSim<sup>®</sup>, the diffusive flux length is divided by the air saturation of the cell for all diffusive flux links in ARM.

$$D_s = \frac{A}{\frac{(L_i/S_{ai})}{d_{ms}\tau_i n_i} + \frac{(L_i/S_{aj})}{d_{ns}\tau_j n_j}} \quad (9)$$

where  $S_{ai}$  is the air saturation within cell  $i$ . This makes the two flux calculations consistent.

### 3.5 Radon

Utilizing decay chain data found in the radionuclide data package (SRNL Radionuclide, Element and Dose Parameters Data Package\_12-30-15\_version 1.1), 86 decay chains of varying length were found that lead to Rn-222. It was decided to screen out parents upstream of U-238 due to its primordial half-life, which eliminates over half of the 86 chains. A decision was also made to utilize a half-life screening criterion of at least one day, which results in the addition of nine Rn-222 parents (Cf-246, Am-242m, Am-242, Cm-242, Np-234, Np-238, Pa-230, Pa-234m, and Th-234) to the previous five (U-238, U-234, Th-230, Ra-226, and Pu-238) that were studied in the 2008 E-Area PA (WSRC, 2008). Th-234 and Pa-234m were dismissed in 2007 because of their shorter half-lives. In total, six decay chains are included in the ARM as shown below and in Figure 3-1, where the colored numbers correspond with the following decay chains:

- 1 U-238 -> Th-234 -> Pa-234m -> U-234 -> Th-230 -> Ra-226 -> Rn-222
- 2 Cf-246 -> Cm-242 -> Pu-238 -> U-234 -> Th-230 -> Ra-226 -> Rn-222
- 3 Am-242m -> Am-242 -> Cm-242 -> Pu-238 -> U-234 -> Th-230 -> Ra-226 -> Rn-222
- 4 Am-242m -> Np-238 -> Pu-238 -> U-234 -> Th-230 -> Ra-226 -> Rn-222
- 5 Np-234 -> U-234 -> Th-230 -> Ra-226 -> Rn-222
- 6 Pa-230 -> Th-230 -> Ra-226 -> Rn-222

The Model container, “Inventory,” controls which Rn-222 parent is placed into the waste cells by choosing a number from 1 to 15 as illustrated in Table 3-1.

“Rn\_inventory” determines how much of the parent is placed into the waste cells, and is currently set to 0.25 Ci to account for emanation. The container “Radon” includes the inventory tables for each option of “Inventory.” The inventory tables are used by each unit’s WZ\_inventory switch (found in Model/\*unit type\*/Parameters). The WZ\_inventory switch was modified from the original version to account for the value of “Inventory” by picking which inventory list is used. A snapshot of this element is shown in Figure 3-2.

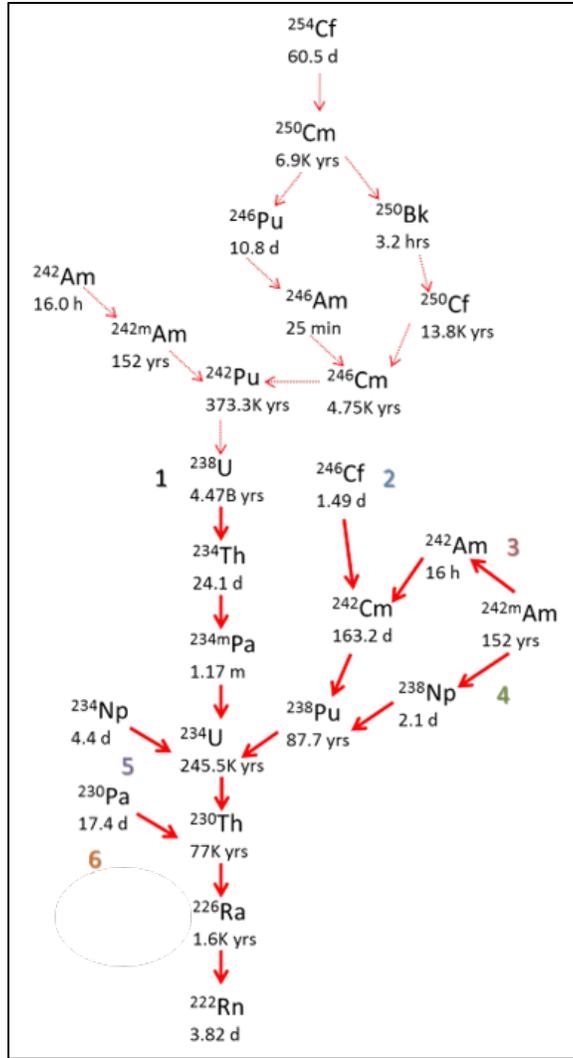
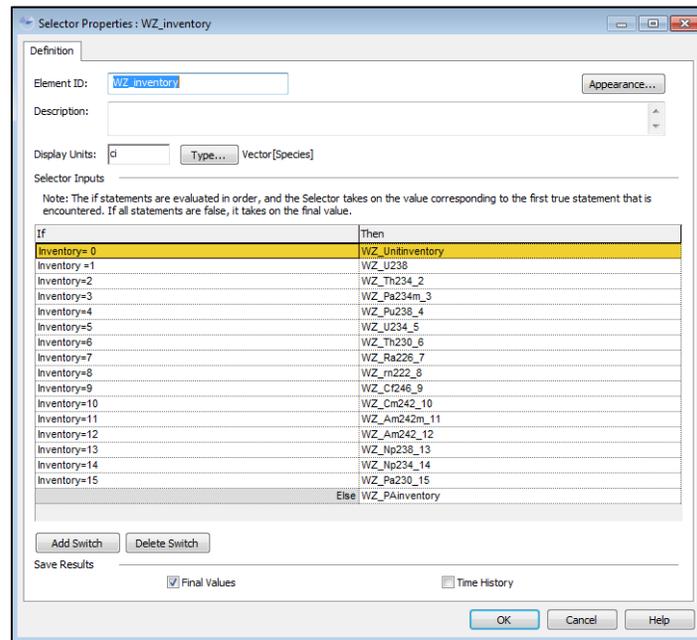


Figure 3-1. Rn-222 decay path with chain parents numbered (the number and color correspond to the decay chain above)

**Table 3-1. Choices for the element “Inventory”**

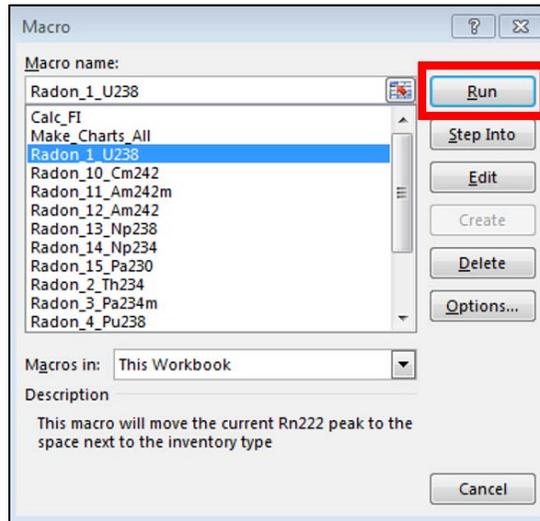
Inventory Number	Parent or Inventory Type
0	Unit Inventory-NON RADON analysis
1	U-238
2	Th-234
3	Pa-234m
4	Pu-238
5	U-234
6	Th-230
7	Ra-226
8	Rn-222
9	Cf-246
10	Cm-242
11	Am-242m
12	Am-242
13	Np-238
14	Np-234
15	Pa-230



**Figure 3-2. The selector properties of WZ\_inventory**

Several Excel macros were created in the Results4.xls workbook to automate the movement of the Rn-222 peak flux and time-of-peak listed for each disposal limit to correspond with the correct parent radionuclide simulated. The simulation outputs the inventory number into the first cell of the worksheet, “Radon,” as well as the Rn-222 peak information for each disposal unit under their respective unit headers. In addition,

the simulation outputs the Rn-222 flux time history for each disposal unit. The macros transfer the Rn-222 time history for each disposal unit to their respective worksheet under the parent radionuclide. First, ensure that you enable macros when you open Results4.xls. To run the macro: under “Macros” in the “View” bar, choose “View Macros” and pick the correct macro for the inventory number (1 to 15) then press “Run”, as shown in Figure 3-3. The macro “Calc\_FI” automates the fraction of inventory calculation.



**Figure 3-3. Macro screen shot showing the naming convention of each macro**

For example, if the inventory number is 1 (U-238), choose “Radon\_1\_U238.” After the macro execution completes, be sure to save Results4.xls.

### 3.6 Material Database

A Microsoft Access material database was created that contains all material properties (each material’s porosity, water saturation, and bulk density) utilized within the ARM. The database also reports the reference for each property value within the “Description” column (these include: Phifer, 2003; Phifer, 2006; WSRC, 2008; and Hiergesell, 2011). Note that if statistics are not available, as is the case for both the waste and cap materials, the standard deviation is set to 0.1, the minimum value is 0.05 less than the deterministic value, and the maximum is 0.05 more than the deterministic value. An exception to this rule applies for water saturation of some waste materials (LAWV, ILV, and NRCDA) that are regarded as “dry” (see Table 7-1 by WSRC, 2008). In these cases, the mean, standard deviation, minimum, and maximum water saturation values were set to 1E-05, 0.01, 1E-06, and 1E-04, respectively.

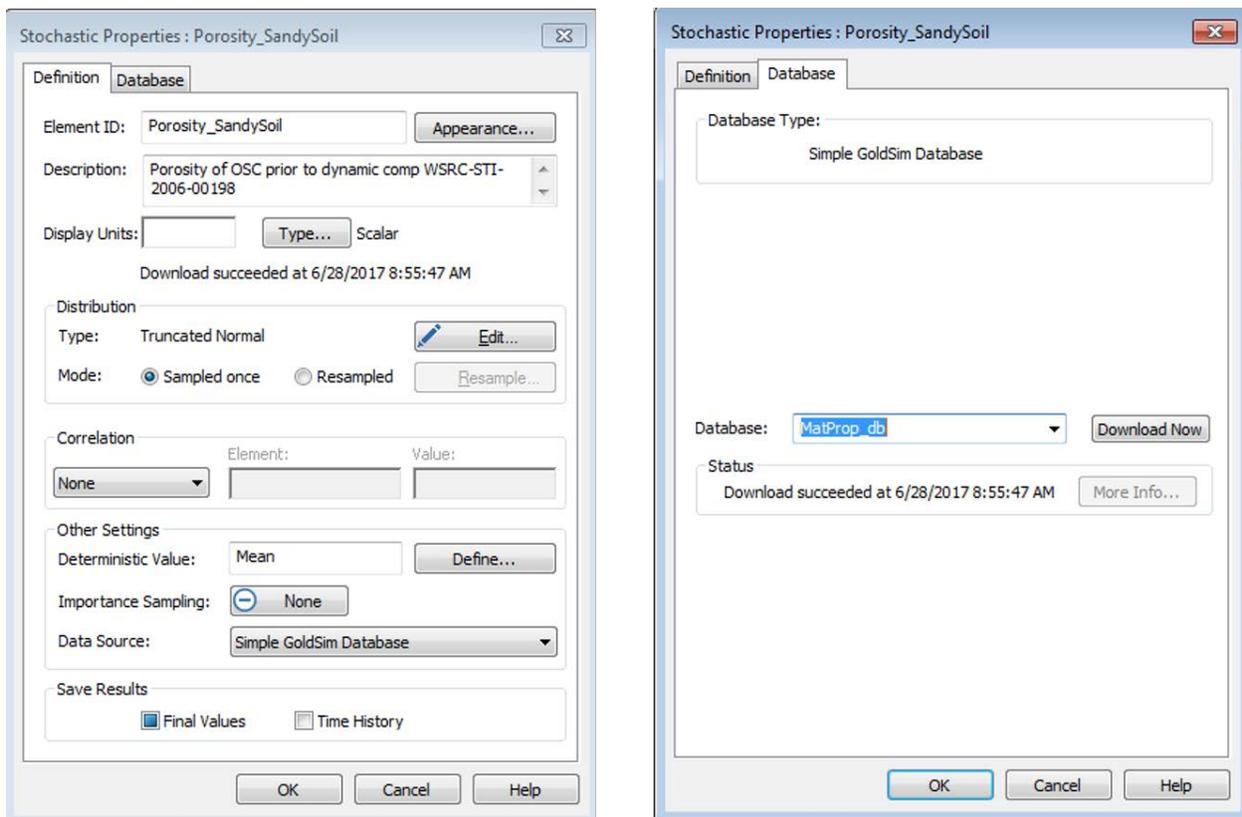
To link the Microsoft Access material database with the GoldSim® stochastic element, the material database must first be added as a data source using the Data Sources 32-bit ODBC administrator (type ODBC in the search box at the bottom of the Windows Start Menu and choose the 32-bit option). In the ODBC Data Source Administrator menu, select Add and then choose the Microsoft Access Driver (\*.mdb, \*.acdb). On the Setup screen, type in the Data Source Name (in this case, MatProp\_db), click the ‘Select’ button under Database, and finally locate MatProp\_db.acdb within the computer’s directories. Once completed, be certain to keep the most up-to-date Access database in the specified subdirectory.

Each stochastic element related to material properties is modified by choosing the “Simple GoldSim Database” option as its Data Source (see Figure 3-4). On the Database tab, MatProp\_db is then selected as the Database as shown in Figure 3-4. After each stochastic element is edited (and after any database modifications are performed), select MODEL from the main menu, then Database, and finally Database Download.

### 3.7 Material Container

The following improvements were implemented:

- Modified “Atmosphere” fluid properties to be consistent with calculated Henry's Law constants (UnitlessHenry) and provided a Reference Diffusivity of D0radon (the open-air diffusion coefficient for Rn-222) and Relative Diffusivities of SqrtMolWtRatio. Multiplying the reference diffusivity by the relative diffusivity of each species will result in the open-air diffusion coefficient for each radionuclide.
- Modified the soil element, “SandySoil,” to link to Dry (bulk) Density and Porosity found in the SandySoilProperties container instead of using a typed-in value. The cap material properties (found in /Model/Material/Cap\_Materials) were also altered to link with elements in their respective stochastics containers (and therefore link to the database).



**Figure 3-4. Stochastic element property menus (left window shows where to select the type of Data Source used; right window shows where to select the Database Name)**

### 3.8 Henry's Law Constants

Henry's Law constants utilized by GoldSim® in the calculation of solute concentration were updated per Dyer (2017) for the volatile radionuclides included in the 2017 ARM. At pH 5.4, Hg-194 and Hg-203 can exist as HgCl<sub>2</sub>, Hg<sup>0</sup>, or both depending on redox conditions. To be conservative, the dimensionless Henry's Law constant for the more volatile Hg<sup>0</sup> species was used. The new Henry's Law constants as well as those from the 2011 ARM are listed in Table 3-2. The values shown for soil pH 5.4 are found in the data element "UnitlessHenry\_JD," while the values shown for soil pH 8.23 (cells having cementitious materials) are found in the data element "UnitlessHenry\_JD\_Concrete."

**Table 3-2. Dimensionless Henry's Law Constants used in ARM.**

Elemental Isotope	Dimensionless H <sub>i</sub> Soil at pH 5.4 (molar vapor/molar liq.)		Dimensionless H <sub>i</sub> Soil at pH 8.23 (molar vapor/molar liq.)	
	2011 ARM	NEW	2011 ARM	NEW
Ar39	N/A	29	N/A	29
C14	1.097	1.1	0.9998	0.015
Cl36	8.02E-14	7.90E-14	1.16E-16	1.10E-16
H3	1.99E-05	1.90E-05	1.99E-05	1.90E-05
I129	6.62E-17	6.50E-17	3.21E-31	3.10E-31
Kr85	N/A	17	N/A	17
Ra226	3.40E+38	1.00E-30	3.40E+38	1.00E-30
Rn222	3.40E+38	4.5	3.40E+38	4.5
S35	3.40E+38	9.40E-06	3.40E+38	1.03E-09
Sb124	6.04E-35	5.90E-35	0	8.30E-41
Sb125	6.04E-35	5.90E-35	0	8.30E-41
Se75	1.49E-27	1.50E-27	0	1.10E-89
Se79	1.49E-27	1.50E-27	0	1.10E-89
Sn113	0	4.30E-56	0	6.70E-64
Sn119m	0	4.30E-56	0	6.70E-64
Sn121	0	4.30E-56	0	6.70E-64
Sn121m	0	4.30E-56	0	6.70E-64
Sn123	0	4.30E-56	0	6.70E-64
Sn126	0	4.30E-56	0	6.70E-64
Ar37	N/A	29	N/A	29
Ar42	N/A	29	N/A	29
Kr81	N/A	17	N/A	17
Hg194	N/A	0.32	N/A	8.60E-11
Hg203	N/A	0.32	N/A	8.60E-11
Xe127	N/A	9.4	N/A	9.4

### 3.9 Components-in-Grout (CIG) Trench

CIG grout collapse and cap/waste degradation were implemented in the ARM at 300 years after the end of operations. After year 300 (if start time is at the end of operations), it is assumed that the grout structure encapsulating the waste collapses. This results in settlement of the waste zone and destruction of the closure

cap structure. The waste layer collapses from 14 feet to 7 feet at year 300 (implemented in the data element “Collapse\_time”) per Phifer (2006). This reduction in waste layer thickness is achieved with the same model layout used in prior simulation years by conservatively reassigning the rad inventory of the lower 7 feet of the waste zone to the upper 7 feet of the waste zone.

This reassignment is handled in the container Model/CIG/WasteColumn/MoveInventory. First, the initial 7 feet of waste (from the lower waste zone cells LWZ\_1\_01 to LWZ\_1\_10) is collected into a mass collector element “MassCollector” using a trigger “AddMassFromLWZ.” The trigger definition is set to an elapsed time greater than or equal to the “Collapse\_time” minus 0.01yr (the collapse time is equal to 300 yr + Start\_time where Start\_time is the beginning of institutional control and is set to zero if the simulation begins at year 2040). At this trigger time, each cell in the lower waste zone undergoes a discrete change that zeros out the cell inventory (seen in LWZ\_1\_01 to LWZ\_1\_10 in /Model/CIG/WasteColumn as “ZeroMassInLWZ” in the Discrete Changes section under Cell Inventory). The waste from the collector is then uniformly placed into the upper 7 feet of the waste (UWZ\_1\_01 to UWZ\_1\_10) by the trigger “AddMassToUWZ” (this is imposed in the Discrete Changes section for UWZ cells). The mass flux link was also set to zero between the upper (UWZ\_1\_01) and lower waste zones (LWZ\_1\_10) using the Collapse switch which equals 1 m<sup>2</sup> if simulation time is prior to collapse and 0.0 m<sup>2</sup> (no diffusion) after collapse.

In addition, waste and grout material properties were changed at collapse to those for the E-Area Operational Soil Cover at year 300 (Phifer, 2006). A switch was created for each material property of the waste and grout (dry bulk density, porosity, and water saturation) that toggles between the initial properties (before collapse/degradation) and “OSC prior to dynamic compaction” properties (after collapse/degradation). These switches are found in both /Model/Material/CIG\_WasteProperties (controlled by the data element “Waste\_failure” in /Model/CIG) and /Model/Material/CIGGroutProperties (controlled by the data element “Collapse\_time” in /Model/CIG).

Due to collapse, the closure cap structure is also destroyed; therefore, the hydraulic properties of the cap convert to those of the E-Area Operational Soil Cover (Phifer, 2006). This was achieved by creating a separate container called “Cap\_After\_Collapse” with the same cell number/thickness as the original SRS\_ClosureCap cells, but with material properties equal to those of Sandy Soil (E-Area Operational Soil Cover) and having an \_s\_ added to the cell names (i.e., Erosion\_s\_1 versus original Erosion\_1). Similar to the method used to transfer inventory from the LWZ to the UWZ, the container /Model/CIG/Cap\_After\_Collapse/MoveInventory was created to move inventory from the original closure cap components to those after collapse.

A stochastic element was created (PoreWaterContent\_CIG\_CL) to connect the clean layer water saturation to the database. The total waste thickness was also changed from 16 feet to 14 feet to be consistent with WSRC (2008) by setting data elements “LowerWZThickness\_initial” and “UpperWZThickness\_initial” to 7 feet in /Model/CIG/Parameters. The initial and final (before and after collapse) waste zone thicknesses are equal. In addition, some of the waste cells were comprised of ILV\_concrete instead of CIG\_Waste; this was corrected. In the /Model/CIG/Layering container, each InvAdd(1-4) trigger was changed to place inventory at Start\_Time (previously at year 25 because simulation started at the beginning of operations). For all cells, the diffusional distance of each cell type was modified to take credit for each material’s air saturation in the flux calculations.

### 3.10 Intermediate Level Vault (ILV)

The diffusional distance of each cell type was modified to take credit for each material's air saturation in the flux calculations. The concrete roof thickness was also changed from 24 inches to 27 inches to be consistent with WSRC (2008).

In order to determine if including the special waste forms into ARM is necessary, the H3\_IP2 and H3\_TPB inventory was added to the ILV estimated inventory at closing. It was decided that H3\_IP2 and H3\_TPB were not required to be treated as special waste forms because the preliminary limits produced in the model are orders of magnitude above the total ILV inventory (adding the waste form inventory to the regular waste inventory) at closure (Sink 2016b).

### 3.11 Low Activity Waste Vault (LAWV)

The diffusional distance of each cell type was modified to take credit for each material's air saturation in the flux calculations.

### 3.12 Slit/Engineered Trench

The diffusional distance of each cell type was modified to take credit for each material's air saturation in the flux calculations. The final waste zone thickness after compaction was changed to 2.5 feet to be consistent with the estimates given in WSRC (2008). The diffusive flux link between the top of the clean layer (Cl\_10) and the closure cap was corrected to prevent diffusion to the cap prior to its placement. The diffusive flux link between the first clean layer cell (CL\_1) and the second clean layer cell (CL\_2) was also corrected (in /Model/Slit); the previous model eliminated diffusion between these layers after compaction.

### 3.13 Naval Reactor Component Disposal Area

The 2011 version of ARM did not divide the NRCDA source inventory by the number of waste cells; therefore, the model used 1 Ci inventory (times the corrosion rate) for each waste cell (giving a total of 5 Ci). Dividing the inventory by the number of waste cells (so there is a total of 1 Ci distributed evenly among the 5 waste cells) results in an order-of-magnitude increase in NRCDA C-14 limits.

Another significant change was to implement the rate of radionuclide release as described in the Special Analysis (SA) of the Naval Reactor Waste Disposal Pad (Yu et. al., 2002) and also implemented in the 2008 E-Area PA (WSRC 2008). In the 2011 ARM, the corrosion of activated metal components was assumed to be equal to that of the stainless-steel cask. Thus, once the cask weld was breached, radionuclides were assumed to be released into the surrounding soil at a rate controlled by this corrosion rate (0.004 Ci/yr). The 2002 SA, however, specifies that a representative activated metal component consists of the corrosion resistant metal alloys Inconel and Zircaloy which have much smaller corrosion rates than stainless steel.

There is no standard Naval Reactor waste container due to the variety of Naval Reactor waste components. Detailed configurational descriptions of the Naval Reactor waste components are not available because of the classified nature of this information. According to data supplied by the Naval Reactor program, a representative type of activated waste component is the Knolls Atomic Power Laboratory (KAPL) core barrel/thermal shield (CB/TS). The KAPL CB/TS was used to represent the various types of activated metal components in the 2002 SA and 2008 PA as the majority of the activity projected for the 643-26E NRCDA will be contained in this type of component. The KAPL unit is comprised of six component parts, four

made of Inconel and two of Zircaloy. Radionuclides are distributed between the two alloys unequally. Of the 24 radionuclides of interest in the most recent air pathway and radon screening study (Dyer 2017), only the distribution of C-14 is documented in the SA (88 % in Zircaloy and 12 % in Inconel). To be conservative, all other radionuclides are modeled to exist entirely in Inconel since it has the higher effective corrosion rate of  $5 \times 10^{-5}$  cm/yr compared to  $5 \times 10^{-6}$  cm/yr for Zircaloy. The rate of release of a given radionuclide is shown in Equation (10).

$$Rate\_Release = I_A \left( f_I \sum_{i=1}^{i=4} I_i C_i + f_Z \sum_{i=5}^{i=6} I_i C_i \right) \quad (10)$$

Where  $I_A$  is the inventory of the radionuclide of interest;  $f_I$  and  $f_Z$  are the fraction of the radionuclide inventory in the Inconel and Zircaloy metal alloys, respectively;  $I_i$  is the fraction of the component part,  $i$ , in the total alloy;  $C_i$  is the fraction of the component part,  $i$ , corroded per year. Since the inventory is handled in a separate model element, the rate of release has the units  $y^{-1}$  and is multiplied by the inventory in each waste cell in the elements “rate\_initial\_inventory” and “SourceRate\_1” depending on if decay is turned on or off (discussed below). This modification, when implemented in the PA, will lead to at least two orders-of-magnitude increase in the disposal limit for C-14 established in the 2011 Air Pathway SA (Hiergesell 2011).

The 2011 ARM version does not deposit the inventory into the NRCDA casks until they are breached at year 750. In order to be consistent with the other units as well as take credit for decay, a single cell (initial\_inventory) was created in /model/NRCDA/Parameters. It has an initial inventory of WZ\_inventory / Species.Specific\_Activity and has no flux links to other cells in the model. The input “NRCDA\_Source” enables the user to choose to not allow decay prior to cask failure (with a value of 1) or to allow decay prior to failure by choosing a value of 2. If decay is implemented, the inventory deposited into the waste stream is equal to the radionuclide mass in the cell initial\_inventory at the time of cask failure.

### 3.14 Closure Cap

Modifications were made in all disposal unit containers (/Model/\*unit\*/SRS\_ClosureCap). Closure cap cell parameters were modified to coincide with the proposed final cover design as well as to take credit for partial air saturation in the flux calculation. The modifications are outlined in Table 3-3.

Every erosion barrier (EB) cell in each disposal unit cap container (Erosion\_1 through Erosion\_4 in the container /Model/\*unit\*/SRS\_ClosureCap/CapCells) was modified. In the 2011 version, the cells were comprised of Consolidated Low Strength Material (CLSM) instead of EB and utilized the porosity and dry bulk density of CLSM when defining the amount of each media (soil, water, air) within each cell (Equation (11)). The CLSM medium was deleted from each cell and replaced with EB. “Porosity\_EBarrier” ( $\eta$  in Equation (11)) and “DryBulkDensity\_EB” ( $\rho_d$  in Equation (11)) were then utilized for defining the media quantities. In Equation (11),  $VM_{soil}$  is the mass quantity of soil (M),  $VM_{water}$  and  $VM_{air}$  are the volumes of water and air, respectively ( $L^3$ ),  $S_w$  is the water saturation, and  $S_a$  is air saturation.

$$\begin{aligned} VM_{soil} &= V_{cell} * \rho_d \\ VM_{water} &= V_{cell} * n * S_w \\ VM_{air} &= V_{cell} * n * S_a \end{aligned} \quad (11)$$

**Table 3-3. Cap elements modified in 2017 ARM**

Element Name	2011	2017	Reason
EB_Cell_Vol	EB_CellThickness*Unit Area *Cobble_Porosity	EB_CellThickness*UnitArea	EB cells now utilize Ebarrier stochastics instead of CLSM
EB_DiffDist	EB_CellThickness/2	EB_CellThickness/(2*EB_AirResidSat)	Properly account for air saturation in flux calculation
EB_ResidSat	0.825	ResidSat_EB	Link to Material Database
GeoTxt_DiffDist	LCCB_CellThickness/2	GeoTxt_CellThickness/(2*UCCB_AirResidSat)	Properly account for air saturation in flux calculation
GeoTxt_NumberCells	4	2	Only 2 cells in model
GeoTxt_ResidSat	0.7	GeoTxt_Stochastics.ResidSat_GeoTxt	Link to Material Database
GeoTxt_Thickness	1 foot	0.2 inches	To be consistent with cap design
Gravel_DiffDist	Gravel_Thickness/2	Gravel_CellThickness/(2*Gravel_AirResidSat)	Properly account for air saturation in flux calculation
Gravel_ResidSat	0.7	ResidSat_Gravel	Link to Material Database
GTClay_DiffDist	GTClay_CellThickness/2	GTClay_CellThickness/(2*GTClay_AirResidSat)	Properly account for air saturation in flux calculation
GTClay_ResidSat	0.7	ResidSat_GeoTxt_Clay	Link to Material Database
GTClay_Thickness	2 inches	0.2 inches	To be consistent with cap design
LCCB_DiffDist	LCCB_CellThickness/2	LCCB_CellThickness/(2*LCCB_AirResidSat)	Properly account for air saturation in flux calculation
LCCB_ResidSat	0.7	ResidSat_CCBbackfill	Link to Material Database
UCCB_DiffDist	UCCB_CellThickness/2	UCCB_CellThickness/(2*UCCB_AirResidSat)	Properly account for air saturation in flux calculation
UCCB_ResidSat	0.7	ResidSat_CCBbackfill	Link to Material Database

Previously, to account for the difference in porosity, the element “Cobble\_Porosity” (which is approximately Porosity\_EBarrier/Porosity\_CLSM) was used in the cell volume calculation. Although this eliminates incorrect usage of CLSM’s porosity instead of the porosity of the EB to calculate the quantity of each media within the cell, the defined soil’s porosity (in 2011 this was CLSM) through which the volatile radionuclides are diffusing is also utilized in calculating the diffusive conductance as shown in Equation (8). Therefore, when CLSM was used for the soil media, its porosity was influential in the flux calculation. Changing the media to EB with its much smaller total porosity increases inventory limits for those radionuclides that have a peak dose after closure cap.

The fifth cell in the lower controlled compacted backfill layer, LCB\_5, was also modified. The 2011 version assumed 0.0 m<sup>3</sup> for the water volume; this was changed to LCCB\_Cell\_Vol\*CCBackfill:Porosity\*LCCB\_ResidSat in the new version. The gravel cells were also corrected in the new version. The 2011 version used the air saturation to define the water volume and water saturation to define the air volume. Finally, the GeoTxt cells were modified in the new version because the incorrect cell volume was used in the 2011 ARM.

#### 4.0 References

- Butcher, B. T. and Phifer, M. A. 2016. *Strategic Plan for Next E-Area Low-Level Waste Facility Performance Assessment*. SRNL-STI-2015-00620, Revision 0. February 2016.
- Dixon, K. L. and Moore, K. R. 2017. *Air Pathway Dose Modeling for the E-Area Low-Level Waste Facility*. SRNL-STI-2016-00512, Revision 1. September 2017.
- Dyer, J. A. 2017. *Recommended Henry's Law Constants for Non-Groundwater Pathways Models in GoldSim*. SRNL-STI-2017-00331, Revision 0. June 2017.
- Dyer, J. A. 2017. *Air and Radon Pathways Screening Methodologies for the next Revision of the E-Area PA*. SRNL-STI-2017-00568, Revision 0. November 2017.
- Flach, G. P., Kaplan, D. I., Nichols, R. L., Seitz, R. R., and Serne, R. J. 2016. *Solid Secondary Waste Data Package Supporting Hanford Integrated Disposal Facility Performance Assessment*. SRNL-STI-2016-00175, Revision 0. May 2016.
- GTG. 2017. *GoldSim® User's Guide Version 12.0*. GoldSim® Technology Group. Issaquah, WA. February 2017.
- Hiergesell, R. A. and Taylor, G. A. 2011. *Special Analysis Air Pathway Modeling of E-Area Low-Level Waste Facility*. SRNL-STI-2011-00327, Revision 0. August 2011.
- Phifer, M. A. 2003. *Saltstone Disposal Facility Mechanically Stabilized Earth Vault Closure Cap Degradation Base Case: Institutional Control to Pine Forest Scenario (U)*. WSRC-TR-2003-00523, Revision 0. December 2003.
- Phifer, M. A., Millings, M. R., and Flach, G. P. 2006. *Hydraulic Property Data Package for the E-Area and Z-Area Soils, Cementitious Materials, and Waste Zones*. WSRC-STI-2006-00198, Revision 0. September 2006.
- Sink, D. F. 2016a. *FY16 SWMF Low Level Waste Plan and Disposal Strategies*. SRNS-RP-2016-00162, Revision 0. April 2016.
- Sink, D. F. 2016b. "EAV Low Level Waste Facilities – Projected Radionuclide Inventories at Closure". SRNS-N4222-2016-00007, Revision 0. May 16, 2016.
- WSRC. 2008. *E-Area Low-Level Waste Facility DOE 435.1 Performance Assessment*. WSRC-STI-2007-00306, Revision 0. Washington Savannah River Company. Aiken, SC. July 2008.
- Yu, A. D., McDowell-Boyer, L. M., Cook, J. R., Young, K. E. 2002. *Special Analysis: Naval Reactor Waste Disposal Pad (U)*. WSRC-RP-2001-00948, Revision 2. December 2002.

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