ENGINEERING CALCULATIONS AND ANALYSIS REPORT

Title: Air Pathway Assessment for the INL Remote-Handled Low-Level Waste Disposal Project

ECAR No.: 1370 ECAR Rev. No.: 1 Project File No.: NA Date: 09/28/2011

1. Index Codes
   Building/Type: NA SSC ID: NA Site Area: NA

2. Quality Level and Determination No.: QL-2 (#MSA-000136)

3. Objective/Purpose:
   The purpose of this report is to document an assessment of potential emissions of gaseous radionuclides from the proposed Idaho National Laboratory Remote-Handled Low-Level Waste Disposal Facility. It includes an evaluation of the potential release and transport of gas-phase radionuclides (excluding radon) from the facility to a hypothetical receptor via the air pathway and compares predictions of dose to a regulatory limit of 10 mrem/year. It also includes an evaluation of potential radon surface emissions from the facility for comparison to a regulatory limit of 20 $pCi/m^2/s$. This provides a conservative assessment of the doses and emissions for comparison to regulatory limits during and after the compliance period. Actual doses and radon surface emissions would be expected to be much lower because of the conservative assumptions used in the analysis.

4. Conclusions/Recommendations:
   Based on the results of this assessment, air pathway doses from the proposed Idaho National Laboratory Remote-Handled Low-Level Waste Disposal Facility are expected to be much lower than the allowable standard in 40 CFR 61, Subpart H. Radon fluxes also are expected to be much lower than the allowable standard in 40 CFR 61, Subpart Q.

5. Review (R) and Approval (A) and Acceptance (Ac)[1]:

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1. Review and approval are required. See LWP-10200 for definitions and responsibilities.
2. Electronic Change Request (eCR) numbers in lieu of signatures on this page indicate electronic final review, approval and acceptance by the listed individuals.
3. If required, per LWP-10200.
4. Required if the ECAR contains safety software validation.

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Title: Air Pathway Assessment for the INL Remote-Handled Low-Level Waste Disposal Project

ECAR No.: 1370 ECAR Rev. No.: 1 Project File No.: NA Date: 09/28/2011

SCOPE AND BRIEF DESCRIPTION

Two locations at the Idaho National Laboratory (INL) (shown in Figure 1) are being considered for a proposed remote-handled low-level waste (RH-LLW) disposal facility (Harvego et al. 2010). The purpose of this report is to document an assessment of potential emissions of gaseous radionuclides from the proposed RH-LLW disposal facility. It includes an evaluation of the potential release and transport of gas-phase radionuclides (excluding radon) from the facility to a hypothetical receptor via the air pathway and compares predictions of dose to a regulatory limit of 10 mrem/year (40 CFR 61, Subpart H [2006]; DOE Manual 435.1-1 [2001]). It also includes an evaluation of potential radon surface emissions from the facility for comparison to a regulatory limit of 20 pCi/m^2/s (40 CFR 61, Subpart Q [2006]; DOE Manual 435.1-1 [2001]). This assessment is not meant to provide an estimate of actual doses or radon surface emissions; rather, it is a conservative evaluation to demonstrate that the doses and fluxes are expected to be less than regulatory limits during the compliance period. Per DOE Manual 435.1-1, the compliance period is currently 1,000 years following facility closure.

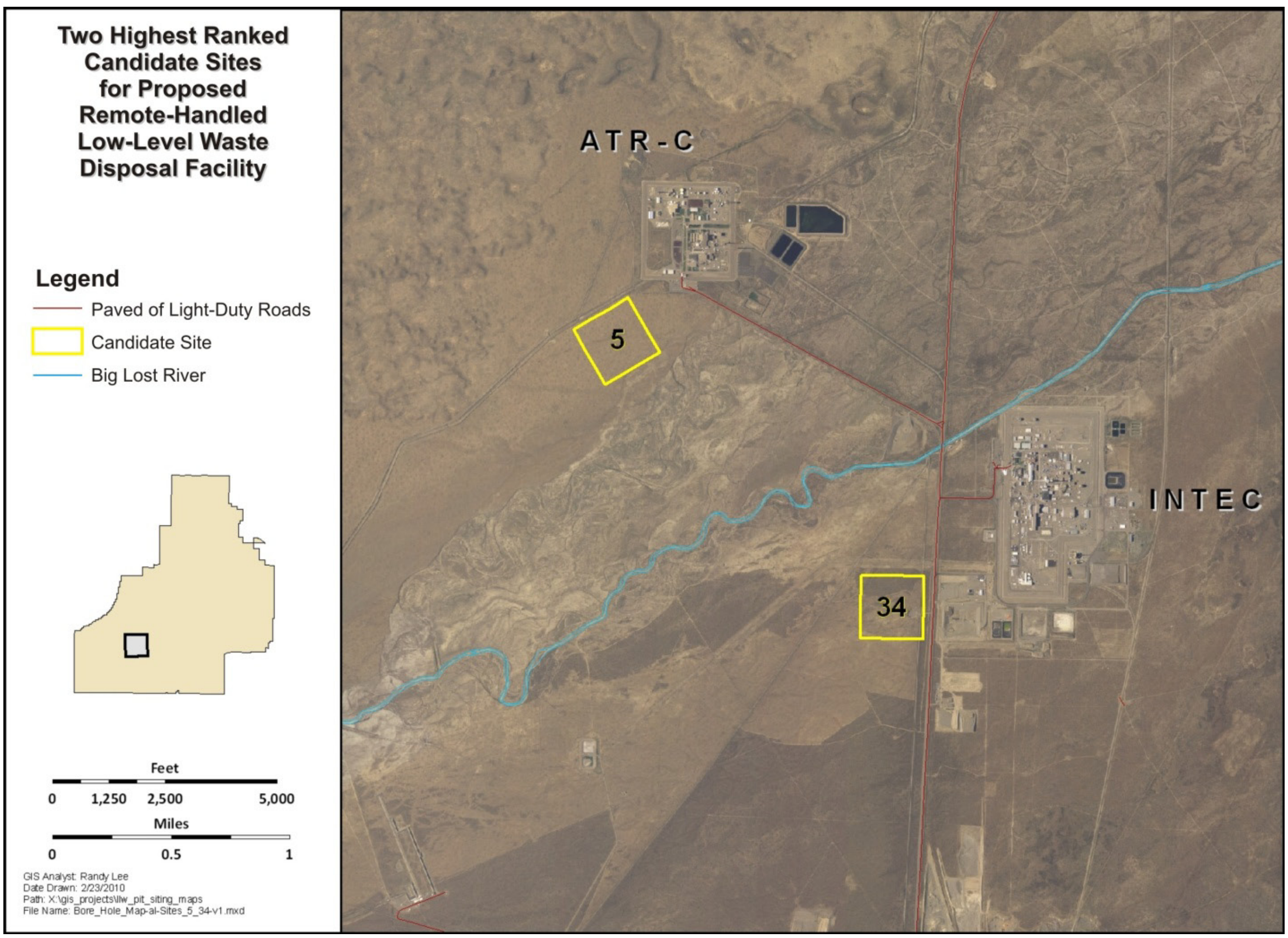

Figure 1. Proposed locations for the Idaho National Laboratory Remote-Handled Low-Level Waste Disposal Facility.

Several models were used in the calculation and assessment of air pathway doses and radon emissions. The U.S. Environmental Protection Agency (EPA) code EMSOFT (EPA 1997) was used to compute the air pathway source term (radionuclide emissions) to the ground surface. The CAP88-PC Version 3 code (EPA 2007) was used to model atmospheric dispersion of volatile radionuclides and doses to potential receptors. Potential radon emissions were modeled using the RESRAD Version 6.4 code (Yu et al. 2001). This ECAR and associated files provide a record that will allow the results to be reproduced if necessary. Electronic files, including spreadsheets, inputs, outputs, and executable files, are provided under "Click here for additional information" (select Supporting Information) in the INL Electronic Document Management System.

DESIGN OR TECHNICAL PARAMETER INPUT AND SOURCES

The following are sources for the primary data used in the assessment:

1. Inventory estimates of all radionuclides were taken from ECAR-851 (2010), ECAR-854 (2010), NRF (2010), ECAR-904 (2010), ECAR-967 (2010) and ECAR-1588 (2011).
2. Ten-year averaged meteorological data (1994 through 2003), gathered at the 10-m elevation of the GRID 3 station located at INL's Central Facilities Area, were used for the CAP88-PC atmospheric dispersion calculations.

References for other data sources are listed in the Discussion/Analysis section.

RESULTS OF LITERATURE SEARCHES AND OTHER BACKGROUND DATA

NA.

ASSUMPTIONS

This section contains a summary of key assumptions used in the analysis. Additional details and other assumptions can be found in the Discussion/Analysis Section.

Air Pathway Assumptions

1. Estimated doses are the result of inhalation of gas-phase radionuclides. Fugitive dust is not a viable pathway because the cover thickness precludes biotic intrusion.
2. All radionuclides from the inventory that are known to exist in the gas phase (excluding radon) were considered for the air pathway. Radon is considered separately.
3. For all calculations, no radioactive decay of the inventory was assumed during the 50-year operational period (i.e., 2108 through 2067).
4. The Phase I screening eliminated radionuclides with half-lives less than 1 year from further consideration.
5. For the Phase II screening calculations, the entire inventory of each radionuclide was transported instantaneously to land surface and released as a gas over a 1-year period. For the 100-m receptor, the inventory was decayed 100 years before being released.
6. For the Phase III screening calculations, radionuclides in activated metals were released by corrosion and transported instantaneously to land surface. Transport of radionuclides in non-activated metals to land surface was simulated using EMSOFT. Assumptions associated with the EMSOFT modeling include the following:
   a. Transport is one-dimensional through a three-layer system consisting of a soil cover, waste zone, and unsaturated sediment. The waste zone is 6-m thick covered by a 1-m thick soil cover with an 18-m thick vadose zone below. All layers have the same properties, but only the waste zone is initially contaminated.
   b. Each radionuclide was modeled as the species that results in the most conservative transport. In this case, C-14 as CO_2 vapor, I-129 as I_2 vapor, and H-3 as both HT and T_2 vapor.

c. Subsurface transport occurs by gaseous diffusion and aqueous advection with linear equilibrium partitioning occurring between the solid, aqueous, and gaseous phases.
d. The pore water flux is steady state based on an infiltration rate of 1 cm/year, the background infiltration rate for undisturbed soils, and greater than the expected rate through the cover.

7. Atmospheric dispersion of radionuclides for the Phase II and III screenings was simulated with CAP88-PC. Assumptions associated with the CAP88-PC dispersion modeling include the following:
   a. All radionuclides were modeled as vapor.
   b. Releases from ground surface were assumed to be from a point source.
   c. The distance from the facility boundary to the INL site boundary is nearly the same for both candidate sites. Therefore, the distance from the Advanced Test Reactor Complex to the site boundary was used in this evaluation to represent the average distance from both facilities.
   d. Doses were calculated for a subsistence-farming scenario, consistent with dose calculations used for the INL Site's annual National Emission Standards for Hazardous Air Pollutants (NESHAP) compliance evaluation (DOE-ID 2010) and reported in terms of the effective dose equivalent.
   e. Average meteorological conditions during the 10-year period from 1994 to 2003 from the 10-m elevation of the GRID 3 station located at the Central Facilities Area were assumed to be representative of future conditions.
   f. Other site-specific and nuclide-specific input parameters were consistent with INL modeling for the annual NESHAP compliance evaluation (DOE-ID 2010).
8. Doses during the 100-year institutional control period (2068 to 2167) were calculated at the INL site boundary in the direction that resulted in the highest dose for the given set of meteorological conditions.
9. Doses after the institutional control period were calculated 100 m from the facility boundary.

Radon Flux Assumptions

1. All radionuclides in the inventory that are sources of radon were considered and include Pu-242, Ra-226, Th-230, U-234, and U-238.
2. Transport from the waste zone through the soil cover is one-dimensional by gaseous diffusion.
3. The soil cover thickness was assumed to be 1 m. This is conservative given the waste zone will be covered with several meters of engineered soil layers upon closure.
4. The radon concentration at land surface is 0 and the bottom boundary is a no-flux boundary, forcing all radon to be emitted at land surface.

COMPUTER CODE VALIDATION

All computer code modeling and spreadsheet calculations in this report were performed on a Dell® Precision Workstation T5400 computer (Intel® Xeon® CPU X5450 @ 3 GHz) running Microsoft® Windows® XP Professional Version 2002 SP3. The computer input files and copies of the spreadsheet worksheets are provided in the appendices. The computer output files are not provided in the appendices due to their size, but are provided on electronic media. All electronic files, including code input, output, executable files, and the spreadsheet files are provided under "Click here for additional information" (select Supporting Information) in the INL Electronic Document Management System.

CAP88-PC Calculations

CAP88-PC Version 3 (EPA 2007) was used to simulate air dispersion of volatile radionuclides for the air pathway assessment. CAP88-PC is one of the codes that EPA allows for demonstration of compliance with the applicable performance objective (40 CFR 61, Subpart H). Additional information about CAP88-PC is located at:

http://www.epa.gov/radiation/assessment/CAP88/aboutcap88.html. The CAP88-PC input files are contained in Appendix A.

EMSOFT Calculations

A modified version of EMSOFT Version 1.3 (EPA 1997) was used to simulate release of volatile radionuclides (not in activated metals) and subsequent transport to land surface. EMSOFT is a computer code used (1) to determine concentrations of contaminants remaining in the soil over a given time, (2) to quantify the mass flux (rate of transfer) of contaminants into the atmosphere over time, and (3) to subsequently calculate contaminant air concentrations by inputting mass flux values into atmospheric dispersion models. In this case, it was only used to quantify mass flux rates. Additional information about EMSOFT, including the source code, can be found at: http://cfpub.epa.gov/ncea/cfm/recordisplay.cfm?deid=2862.

For this air pathway analysis, EMSOFT was modified to bypass the graphical-user interface and allow input of text files. Because of these changes, the modified version of the EMSOFT code was benchmarked with the original version, using the sample problems included in the EMSOFT User's Guide. The comparison yielded identical results, demonstrating the changes were implemented correctly. Appendix B contains the modified EMSOFT source code (Console Version) and the results of the two benchmark problems, including input and output files. Appendix C contains the EMSOFT input files for this air pathway analysis.

RESRAD Calculations

RESRAD Version 6.4 (Yu et al. 2001) was used to estimate radon fluxes at land surface from radon-producing radionuclides in the estimated inventory. The RESRAD code is widely used for deriving limits for radionuclides in soil. It has been verified and undergone several benchmarking analyses. Additional information about RESRAD can be found at: http://web.ead.anl.gov/resrad/home2/. The RESRAD input file is contained in Appendix D.

Microsoft Excel Calculations

Microsoft® Office Excel® 2007 (12.0.6545.5000) SP2 (12.0.6545.5004) was used for several supporting calculations. Portions of the Excel worksheets are copied in Appendix E. To validate the calculations performed with Excel, the formulas in all calculation cells were checked for accuracy and a sample of the calculations were checked by hand.

DISCUSSION/ANALYSIS

Radionuclide Air Pathway Assessment

Analysis Steps

The following steps were used to assess the air pathway. Additional explanation and justification for these steps is provided in the subsequent sections.

1. Identify exposure scenarios.
2. Identify volatile radionuclides in the RH-LLW inventory.
3. Phase I Screening:
    a. Remove radionuclides with half-lives less than 1 year from further consideration. Because of the multi-year operational period, radionuclides with have half-lives less than 1 year will have decayed away to inconsequential levels before or shortly after the facility is closed.

4. Phase II Screening:
   a. For each retained radionuclide, model air dispersion from the RH-LLW disposal facility using the CAP88-PC code. Calculate dose-to-release conversion factors for a unit surface release for both the site boundary receptor and the 100-m receptor.
   b. Estimate surface emissions of the retained radionuclide inventory, assuming the entire inventory is released directly to land surface in 1 year.
   c. Calculate Phase II screening doses for retained radionuclides at both receptor locations by multiplying estimated emissions from Step 4b by the dose-to-release conversion factors from Step 4a.
   d. Apply a Phase II screening threshold of 1 mrem/year, or 1/10 the regulatory limit of 10 mrem/year.
5. Phase III Screening:
   a. For each retained radionuclide, estimate surface emissions for non-activated metals using a more realistic, but still conservative, model accounting for relevant subsurface diffusion, advection, and partitioning processes using the code EMSOFT.
   b. Estimate surface emissions for activated metals assuming corrosion-controlled releases from the activated metals and instantaneous transport to land surface.
   c. Sum the surface emission estimates for non-activated metals from Step 5a and the activated metals from Step 5b for each radionuclide.
   d. Calculate Phase III screening doses for retained radionuclides at both receptor locations by multiplying combined estimated emissions from Step 5c by the CAP88-PC dose-to-release conversion factors from Step 4a.
   e. Sum the Phase III screening doses for each remaining radionuclide and compare to the regulatory limit of 10 mrem/year.

Exposure Scenarios

Air pathway doses were evaluated for receptors most affected by air emissions during the institutional control and compliance periods. During the institutional control period, which begins after closure and lasts for 100 years, the receptor was assumed to be located at the nearest INL Site boundary that yields the highest dose. This receptor is referred to as the site-boundary receptor. After the institutional control period, the receptor was assumed to be located 100 m from a point where all emissions occur from sources at the RH-LLW disposal facility in the direction where meteorological conditions result in the highest air concentrations at that range. This receptor is referred to as the 100-m receptor. Emissions were assumed to be from point sources at ground level for both receptors.

Figure 1 shows the two candidate locations for the proposed RH-LLW disposal facility. Because both locations being considered are approximately the same distance to the INL site boundary and releases (emissions) are expected to be similar for each location, the assessment is considered independent of the two locations.

Source Term Inventory and Phase I Screening

The estimated inventory of radionuclides for a 50-year operating period is summarized in INL (2011a). There are 13 potentially volatile radionuclides in the inventory: Ar-37, Ar-39, Ar-42, C-14, H-3, I-129, I-131, I-132, I-133, Kr-81, Kr-85, Xe-131m, and Xe-133. Of the 13 potentially volatile radionuclides, six (Ar-37, Xe-131m, Xe-133, I-131, I-132, and I-133) have half-lives substantially less than 1 year. Considering that it will take many years to fill this facility with waste, these radionuclides will have decayed away to inconsequential levels before or shortly after the facility is closed (see Table 1). These are not considered in the analysis. Table 2 shows the remaining seven radionuclides and the total estimated inventory for each by waste form.

Tritium (H-3) and C-14 are known to migrate in the gas phase from disposed waste at INL (Koeppen et al. 2006; Fox et al. 2004). Iodine can form gaseous compounds, although it has never been detected in soil pore gas in INL Site disposal areas. Denham, Kaplan, and Yeager (2009) and Denham (2010) researched radioiodine biogeochemistry and determined the primary iodine species that would be present in the vapor phase would be molecular iodine (I_2) and hydrogen iodine (HI). Chemical forms of H-3 include tritiated water vapor (HTO), hydrogen tritium gas (HT) and tritium gas (T_2). Carbon-14 would be transported as carbon dioxide (CO_2). The formation of I_2, HI, and CO_2 depend on the geochemical conditions in the waste and surrounding media. The noble gas isotopes of argon, krypton, and xenon partition only sparingly into the aqueous phase and occur dominantly in gas phase. To ensure that the dose assessment is bounding, it is assumed that geochemical conditions result in gaseous forms that are mobile in the subsurface.

Table 1. Potentially volatile radionuclides with half-lives less than 1 year, which were eliminated from the air pathway analysis.

Nuclide	Half-Life (day)	Total Undecayed Inventory (Ci)	Inventory after 1 year of decay (Ci)
Ar-37	35	1.24E-02	8.92E-06
Xe-131m	11.9	1.42E-10	8.19E-20
Xe-133	5.24	3.34E+04	3.47E-17
I-131	8.04	2.52E+04	5.31E-10
I-132	0.095	5.46E-03	less than 1E-20
I-133	0.87	2.16E-02	less than 1E-20

Table 2. Estimated inventories of potentially volatile radionuclides considered for the air pathway analysis.

Radionuclide	Half-Life (years)	Activated Metal Inventory (Ci)	Non-Metal Inventory (Ci)	Total Inventory (Ci)
Ar-39	269	5.01E-02	0	5.01E-02
Ar-42	33	5.51E-12	0	5.51E-12
C-14	5,730	374	58.5	433
H-3	12.3	3,910	9.84	3920
I-129	1.57E+07	1.33E-05	0.133	0.133
Kr-81	21,000	4.51E-12	0	4.51E-12
Kr-85	10.7	0.938	263	264

Air Dispersion Modeling

The computer code CAP88-PC Version 3 (EPA 2007) was used to model atmospheric dispersion of volatile radionuclides from the RH-LLW facility and dose to a potential receptor. The doses were modeled assuming a subsistence-farming scenario, consistent with dose calculations used for the INL Site's annual NESHAP compliance evaluation. Doses were reported in terms of the effective dose equivalent. The local food production option was selected to simulate a subsistence-farming scenario. Other model parameters were set to CAP88-PC default values, with the exception of I-129 and C-14, which were modeled as vapor (I_2 and CO_2) instead of the particulate form, which is the default form in CAP88-PC for these two radionuclides. The default physical form for the other radionuclides is vapor. Ten-year averaged meteorological data (i.e., 1994 through 2003), gathered at the 10-m elevation of the GRID 3 station located at the INL Central Facilities Area, were used for the calculations. Both locations being considered for the RH-LLW facility are within 4 miles of the station.

Other site-specific and nuclide-specific parameters were obtained from the 2009 INL NESHAP report (DOE-ID 2010). Site-specific parameters include mixing height (800 m); mean temperature (280.2 K); annual precipitation (20.8 cm/year); and absolute humidity (3.54 g/m^3).

Both locations being considered for the RH-LLW disposal facility are approximately the same distance from the INL southern boundary. Because the same meteorological dataset is being used for both facilities, the site boundary results and 100-m results apply to both locations. During the institutional control period, the receptor is at the INL Site boundary at the location of maximum dose. This location is 19.2 km south-southwest of the facility. After institutional control, the receptor is located 100 m from the boundary of the disposal facility. Because a point source was modeled, the modeled receptor distance was the distance from the center of the facility to the edge, plus 100 m.

CAP88-PC was run for a unit release rate (1 Ci/year) to produce dose-to-release conversion factors (mrem/year)/(Ci/year). These conversion factors are presented in Table 3. There are no results for Ar-42 because there is no dose coefficient for Ar-42 in the CAP88-PC nuclide database. Because there is no dose coefficient, the inventory is very small (5.51E-12 Ci), and the half-life is relatively short (i.e., 33 years), this nuclide was not considered further.

Phase II Screening

Prior to estimating the emission rate for each radionuclide using EMSOFT (Phase III screening), a simple and very conservative screening procedure was performed to eliminate inconsequential radionuclides from further analysis using the dose-to-release conversion factors in Table 3. In this process, the total inventory of each radionuclide was released as a gas at land surface over a 1-year period. Doses at both receptor locations were calculated using the dose-to-release conversion factors from the CAP88-PC modeling and compared to a screening threshold effective dose equivalent of 1 mrem/year, which is one-tenth the allowable limit. For the site boundary receptor, the total inventory was released at closure and no credit was taken for releases or decay that may have occurred prior to closure. For the 100-m receptor, the total inventory was decayed 100 years before being released to account for the institutional control period. The results (see Table 4) show the doses are well below the screening threshold for all radionuclides for the site boundary receptor. For the 100-m receptor, only C-14, H-3, and I-129 dose results are above the screening threshold of 1 mrem/year. Surface emissions for these three radionuclides were estimated by simulating subsurface radionuclide transport using the EMSOFT code in the Phase III screening.

Table 3. Dose-to-release conversion factors from the CAP88-PC air dispersion simulations.

Radionuclide	Conversion Factor for Site Boundary Receptor (mrem/year)/(Ci/year)	Conversion Factor for 100-m Receptor (mrem/year)/(Ci/year)
Ar-39	2.2E-08	1.1E-04
Ar-42	None[a]	None[a]
C-14	2.0E-04	1.3E+00
H-3	1.5E-05	8.1E-02
I-129	4.7E-03	2.4E+01
Kr-81	4.7E-08	2.4E-04
Kr-85	4.6E-08	2.4E-04

a. Dose coefficient not available in CAP88-PC database for Ar-42.

Table 4. Phase II screening dose results using the CAP88-PC dose-to-release conversion factors for the site boundary and 100-m receptor locations.

		Site Boundary Receptor			100-m Receptor		
Nuclide	Half-Life (years)	Total Inventory (Ci)	Conversion Factor (mrem/year)/(Ci/year)	Screening Dose (mrem/year)	Total Inventory at 100 Years (Ci)	Conversion Factor (mrem/year)/(Ci/year)	Screening Dose (mrem/year)
Ar-39	269	5.01E-02	2.2E-08	1.1E-09	3.88E-02	1.1E-04	4.4E-06
Ar-42	33	5.51E-12	None	NA	6.74E-13	None	NA
C-14	5,730	433	2.0E-04	8.7E-02	428	1.3E+00	535[a]
H-3	12.3	3920	1.5E-05	5.9E-02	14.0	8.1E-02	1.13[a]
I-129	1.57E+07	0.133	4.7E-03	6.3E-04	0.133	2.4E+01	3.21[a]
Kr-81	21,000	4.51E-12	4.7E-08	2.1E-19	4.49E-12	2.4E-04	1.1E-15
Kr-85	10.7	264	4.6E-08	1.2E-05	0.411	2.4E-04	9.7E-05

a. Screening dose is greater than 1 mrem/year (one-tenth the allowable limit).

Phase III Screening: Emission Modeling using EMSOFT

For radionuclides retained with Phase II screening doses greater than the 1 mrem/year threshold (C-14, H-3 and I-129), a more realistic, but still conservative, method was used to account for subsurface transport. For the portion of the inventory in non-activated metals, the emission rate was estimated, accounting for diffusion, advection, and phase partitioning (including sorption) using the EMSOFT software (EPA 1997). EMSOFT was used to compute the vapor flux (mg/day/cm^2) of C-14, H-3, and I-129 as a function of time at the soil surface for a unit mass concentration (1 mg/kg) in the waste zone. Actual fluxes (emissions) were calculated by multiplying the flux per unit mass concentration from EMSOFT by the actual radionuclide mass concentration in the waste zone. The actual mass concentrations (Ci/kg) were calculated using the non-metal inventories in Table 2, an assumed waste volume of 14,400 m^3 (240 m x 10 m x 6 m) (INL 2011a), and a waste density of 1,820 kg/m^3 (see "EMSOFT Parameter Values" section below). However, the areal dimensions of the facility (240 m × 10 m) have no impact because the fluxes from EMSOFT are multiplied by these dimensions to convert them to a point source.

EMSOFT was not used for the portion of the inventory in activated metals. For activated metals, the emission rate was equal to the rate of release by corrosion and no credit was taken for transport to land surface. In other words, the radionuclides in activated metals are assumed to be transported instantaneously to land surface as they are released from the metal by corrosion. The total emission rate as a function of time from both activated metal and non-metal waste forms were added together and multiplied by the CAP88-PC dose-to-release factors from Table 3 to get the dose estimates at both receptor locations. Site-specific corrosion data from Adler Flitton et al. (2011) were used to estimate the fractional release rate from the activated metal inventory (5.83E-07 1/year; DOE-ID 2011). In both activated and non-activated metal waste forms, no credit was taken for releases or decay that may have occurred during the 50-year operating period prior to closure.

EMSOFT is a one-dimensional model and assumes a steady-state water flux through a homogeneous environment. All layers have the same properties (i.e., bulk density, porosity, moisture content, diffusion coefficients, and partition coefficients [K_d and K_H]). However, each layer may have a different initial concentration. Although the EMSOFT code was written for volatile organic chemicals, the governing equations are appropriate for volatile radionuclides. Contaminants are transported by aqueous advection and aqueous and gaseous diffusion, and they are allowed to partition between the aqueous, gaseous and solid phases. Diffusion can be both upward and downward, but aqueous advection is downward. Aqueous concentrations must be as low as required by the linear equilibrium partitioning assumption. The following summarizes the governing equations discussed in the EMSOFT User's Guide (EPA 1997).

The one-dimensional mass balance equation for a volatile radionuclide that can partition and be transported in the aqueous and gas phases is given by

$$\frac{\partial C_T}{\partial t} = D_E \frac{\partial^2 C_T}{\partial z^2} - V_E \frac{\partial C_T}{\partial z} - \lambda C_T \tag{1}$$

where

C_T = total concentration – total mass of radionuclide per unit volume of soil (Ci/m^3)

D_E = effective diffusion coefficient in the air-filled pore space (m^2/second)

V_E = effective pore water velocity (m/second)

λ = radioactive decay constant (1/second).

The total concentration in soil can be expressed as

$$C_T = \rho_b C_S + \theta C_L + a C_G \tag{2}$$

where

ρ_b = bulk soil density (kg/m^3)

C_S = concentration in the solid phase in soil (Ci/kg)

θ = moisture content

C_L = concentration in the aqueous phase (Ci/m^3)

a = air-filled porosity

C_G = concentration in the gas phase (Ci/m^3).

Using the air-water partitioning relationships (i.e., the Henry's law constant), Equation 2 can be rewritten as

$$C_T = R_S C_S = R_L C_L = R_G C_G \tag{3}$$

$$R_S = \rho_b + \frac{\theta}{K_D} + \frac{a K_H}{K_D} \tag{4}$$

$$R_L = \rho_b K_D + \theta + a K_H \tag{5}$$

$$R_G = \frac{\rho_b K_D}{K_H} + \frac{\theta}{K_H} + a \tag{6}$$

where

K_D = soil-water partition coefficient (m^3/kg)

K_H = dimensionless Henry's law constant.

The Henry's law constant describes the equilibrium partitioning between air and water and is defined by

$$K_H = \frac{P_{vp}}{S} \times \frac{1}{RT} \quad (7)$$

where

P_{vp} = vapor pressure (atm)

S = solubility (mol/m^3)

R = universal gas constant (8.2E-05 atm-m^3/(mol-K))

T = temperature (K).

$$D_E = \frac{K_H D_G + D_L}{R_L} \quad (8)$$

The effective diffusion coefficient is defined by

D_G = soil gas diffusion coefficient = $(a^{10/3}/\varphi^2)\ D_{air}$ (Millington-Quirk model)

D_{air} = the free air diffusion coefficient (m^2/second)

φ = total soil porosity (θ + a)

D_L = liquid diffusion coefficient = $(a^{10/3}/\varphi^2)\ D_{water}$

D_{water} = the diffusion coefficient in water (m^2/second).

The effective pore water velocity is given by

$$V_E = \frac{q}{R_L} \quad (9)$$

where

q = the Darcy velocity in the vadose zone (m/s).

Equation 1 is solved for the boundary conditions

$J(z=0,t) = -hC_g(z=0,t)$

where

J = the volatilization flux across a stagnant boundary layer at the soil surface of depth d (Ci/m^2)

h = the transport coefficient across the boundary layer (m)

C_g = the gas-phase concentration at the surface of the INL RH-LLW Disposal Facility cover (above this layer, the concentration is zero) (Ci/m^3).

$C_T = 0$ *for* $z=\infty$

And the initial condition, $C_T = C_o$ at $t = 0$ from the surface down to some depth L.

The transport coefficient across the boundary layer (h) is defined by

$$h = \frac{D_{air}}{d} \quad (10)$$

where

D_{air} = the free air diffusion coefficient (m^2/second).

The boundary layer thickness (in meters) is estimated by

$$d = \frac{26\upsilon}{0.01V(6.1 + 0.63V)^{0.5}(D_{air}/\upsilon)^{1/3}} \tag{11}$$

where

υ = kinematic viscosity of air (1.5E-05 m^2/second)

V = ambient wind speed (3.22 m/second).

The solution to Equation 1 is given as:

$$\begin{aligned} C_T(z,t,L) &= \frac{1}{2}C_o \exp(-\lambda t)\left[\operatorname{erfc}\left(\frac{z\text{-}L\text{-}V_E t}{2\sqrt{D_E t}}\right) - \operatorname{erfc}\left(\frac{z\text{-}V_E t}{2\sqrt{D_E t}}\right)\right] \\ &+ \frac{1}{2}C_o \exp(-\lambda t)\left[1 + \frac{V_E}{H_E}\right]\exp\left[\frac{V_E z}{D_E}\right]\left[\operatorname{erfc}\left(\frac{z + L + V_E t}{2\sqrt{D_E t}}\right) - \operatorname{erfc}\left(\frac{z + V_E t}{2\sqrt{D_E t}}\right)\right] \\ &+ \frac{1}{2}C_o \exp(-\lambda t)\left[2 + \frac{V_E}{H_E}\right]\exp\left[\frac{H_E(H_E + V_E)t + (H_E + V_E)z}{D_E}\right] \\ &\times \left[\operatorname{erfc}\left(\frac{z + (2H_E + V_E)t}{2\sqrt{D_E t}}\right) - \exp\left[H_E\frac{L}{D_E}\right]\operatorname{erfc}\left(\frac{z + L + (2H_E + V_E)t}{2\sqrt{D_E t}}\right)\right] \end{aligned} \tag{12}$$

The volatile flux at the soil surface is:

$$\begin{aligned} J_s(t,L) &= \frac{1}{2}C_o \exp(-\lambda t)V_E\left[\operatorname{erfc}\left(\frac{V_E t}{2\sqrt{D_E t}}\right) - \operatorname{erfc}\left(\frac{L + V_E t}{2\sqrt{D_E t}}\right)\right] \\ &+ \frac{1}{2}C_o \exp(-\lambda t)[2H_E + V_E]\exp\left[\frac{H_E(H_E + V_E)t}{D_E}\right] \\ &\times \left[\operatorname{erfc}\left(\frac{L + (2H_E + V_E)t}{2\sqrt{D_E t}}\right)\exp\left[H_E\frac{L}{D_E}\right]\text{-}\operatorname{erfc}\left(\frac{(2H_E + V_E)t}{2\sqrt{D_E t}}\right)\right] \end{aligned} \tag{13}$$

Equation 13 gives the flux at the surface for a single contaminated layer of thickness L and no clean cover over the contaminated layer. The solution for an arbitrary number of contaminated layers is obtained through applying the principles of superposition. For n layers of thickness D_i and overlain with a clean cover of thickness DB_i, the total concentration as a function of depth and time is:

$$C_{BT}(z,t) = \sum_{i=1}^{n}\left[C_T(z,t,D_i + DB_i) - C_T(z,t,DB_i)\right] \tag{14}$$

<u>EMSOFT Parameter Values</u>

Figure 2 illustrates the simplified geometry of the one-dimensional EMSOFT model domain for the RH-LLW disposal facility. The cover in the model is assumed to be 1 m of topsoil. The actual thickness of the final cover will likely be several meters thick; therefore, this is a very conservative assumption. The waste zone is 6 m thick and the vadose zone below the waste zone is 18 m thick, which is approximately equal to the cumulative thickness of surface alluvium and sedimentary interbeds between the bottom of the waste zone and the water table. However, because the bottom boundary is a no-flux boundary, all the radionuclides eventually end up as gaseous surface emissions.

The soil porosity (0.32) and bulk density (1.82 g/cm^3) for the EMSOFT simulations are based on the properties of the uppermost soil layer in the proposed ICDF cover design (EDF-9917). The moisture content (0.073) is based on an infiltration rate of 1 cm/year, which is the estimated background infiltration rate for undisturbed soils at the INL site (Cecil et al. 1992).

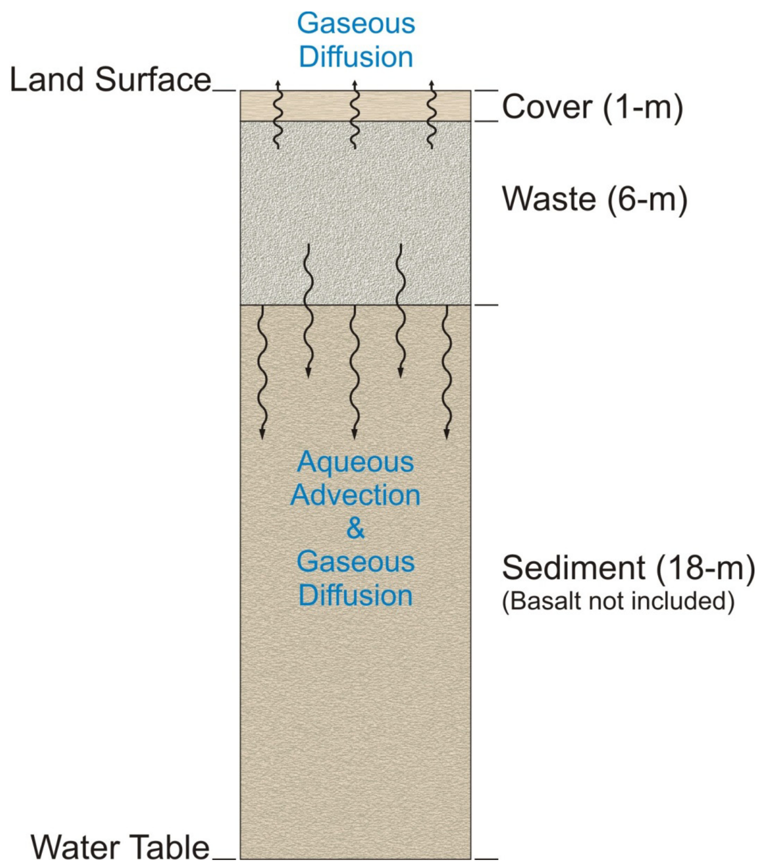

Figure 2. EMSOFT model geometry and primary transport processes.

Radionuclide-specific inverse Henry's law constants are presented in Table 5 and soil-water partition (sorption) coefficients in Table 6. Diffusion coefficients in air and water are shown in Table 7. Sorption coefficients are the recommended values for surface alluvium not impacted by cement leachate (INL 2011b). The inverse Henry's law constants were obtained from Sander (2010) and Denham (2010), who provided inverse Henry's law constants for different geochemical conditions in grouted tank waste at the Savannah River Site. Rationale for selection of the Henry's law constant is provided below:

C-14 CO_2 is the only gaseous form of C-14 considered. Denham (2010) provides inverse Henry's law constants of 2.8 and 0.038 mol/kg-atm for pH environments of 8.3 and 5.4, respectively. Given the neutral to elevated pH of the RH-LLW environment, the value of 2.8 mol/kg-atm was selected.

I-129 Sander (2010) provides a value for I_2 between 1.1 and 3.3 mol/L-atm. However, these are at ideal conditions for the formation of I_2, and Denham, Kaplan, and Yeager (2009) shows that I_2 is unlikely to be stable in pH conditions of greater than about 4 (Figure 6 on page 24 of Denham, Kaplan, and Yeager 2009). Given the neutral-to-elevated pH of the RH-LLW environment, the formation of I_2 is not expected; instead, HI is likely to be the dominant iodine species. The inverse Henry's law constants for HI calculated by Denham (2010) are many orders of magnitude higher than the Sander (2010) value for I_2; this essentially eliminates iodine exposure via the air pathway because very little iodine will exist in the vapor phase. However, for atmospheric dose calculations, I_2 was conservatively assumed to be the dominant species and an inverse Henry's law constant of 1.1 mol/L-atm was used.

H-3 For transport calculations, HT and T_2 were assumed to be the dominant tritium species. HT and T_2 have lower inverse Henry's law constants and higher air diffusion coefficients than HTO, resulting in more vapor-phase partitioning and rapid transport via gas diffusion to the surface.

Table 5. Radionuclide-specific inverse Henry's law values for the EMSOFT simulation.

Chemical Form	Inverse Henry's Law Value (H)	Dimensionless Henry's Law (K_H)	Reference
CO_2	2.8E+00 mol/atm-kg[a]	1.51E-02	Denham (2010) for pH 8.3, Eh 0.73 V
CO_2	3.8E-02 mol/atm-kg	1.11E+00	Denham (2010) for pH 5.4, Eh 0.37 V
I_2	1.1E+00 to 3.3E+00 mol/atm-L[b]	3.84E-02 to 1.263E-02	Sander (2010)
I_2	1.3E+29 mol/atm-kg	3.25E-31	Denham (2010) for pH 8.3, Eh 0.73 V
HI	6.3E+14 mol/atm-kg	6.71E-17	Denham (2010) for pH 5.4, Eh 0.37 V
HT, T_2	7.8E-04 mol/atm-L[c]	5.42E+01	Sander (2010)
HTO	2.1E+03 mol/atm-kg	2.01E-5	Denham (2010)

a. The value used for CO_2 in EMSOFT because the pH is likely to be closer to 8.3 than 5.4.
b. The value used for I_2 in EMSOFT was 1.1 mol/atm-L. This was the most conservative value for vapor-phase transport.
c. The value used for HT and T_2 in EMSOFT. This value is the most conservative for vapor-phase transport of H-3
CO_2 = carbon dioxide
I_2 = molecular iodine
HI = hydrogen iodine
HT = hydrogen-tritium gas
HTO = tritiated water
T_2 = tritium gas

Conversion of the dimensional Henry's law constant to the dimensionless quantity is given by

$$K_H = \frac{1}{H\rho_w RT} \qquad (15)$$

where

H = dimensional inverse Henry's law constant (mol/kg-atm)

ρ_w = density of water (1 kg/L)

R = universal gas constant (8.2E-05 atm-m^3/(mol-K))

T = assumed temperature in the facility (288.5 K).

If the dimensional inverse Henry's law constant is in units of mol/L-atm, then the density of water is omitted in Equation 15.

Table 6. Radionuclide-specific soil-water partition (K_D) coefficients.

Radionuclide	K_D (mL/g)	Reference
C-14	0.5	INL (2011b), recommended value for alluvium
H-3	0	INL (2011b), recommended value for alluvium
I-129	3	INL (2011b), recommended value for alluvium

Table 7. Radionuclide-specific diffusion coefficients in air and water for EMSOFT diffusion simulation for the air pathway. Diffusion coefficients were based on a temperature of 15°C (60°F).

	Diffusion Coefficient		
Chemical Form	(cm^2/second)	(cm^2/day)	Reference
CO_2 (D_{air})	1.53E-01	1.32E+04	EPA (2010)
HT, T_2 (D_{air})	7.94E-01	6.86E+04	EPA (2010)
I_2 (D_{air})	8.71E-02	7.53E+03	EPA (2010)
CO_2 (D_{water})	1.55E-05	1.34E+00	EPA (2010)
HT, T_2 (D_{water})	3.52E-05	3.04E+00	EPA (2010)
I_2 (D_{water})	9.06E-06	7.83E-01	EPA (2010)

CO_2 = carbon dioxide
HT = hydrogen-tritium gas
I_2 = molecular iodine
T_2 = tritium gas

Phase III Air Pathway Dose Estimates

The air pathway results for C-14, H-3, and I-129 are presented in Table 8 and Figure 3. Doses during and after the institutional control period are expected to be well below the 10 mrem/year dose limit required by 40 CFR 61, Subpart H and DOE Manual 435.1-1 at the INL site boundary. The screening calculations provide a conservatively estimated peak total dose of 1.5E-03 mrem/year occurring in year 2068, immediately after closure. The estimated peak total dose after the institutional control period (6.6E-02 mrem/year) occurs in year 2168, 100 years after closure. In both cases, C-14 is the major contributor to the total dose and most of the dose comes from the non-activated metal portion of the inventory. This occurs even though releases from activated metals are assumed to be transported to land surface instantaneously and the non-activated metal portion of the inventory is only 14% of the total for C-14. This is due to the slow corrosion of activated metals and the correspondingly slow release.

Although the dose estimates in Table 8 are much lower than the required limit, the actual doses can be expected to be even less than those in Table 8 because of several conservative assumptions used. This analysis assumed the entire inventory of each radionuclide would eventually be transported to land surface. In addition, no credit was taken for the steel waste containers and concrete vaults in limiting release and transport. The engineered cover also will provide a much longer diffusive pathway than the 1 m of soil used, which will lower doses and shift the peak dose out later in time.

Table 8. Maximum air pathway effective dose equivalent for both receptor locations.

Radionuclide	Receptor Dose at INL Site Boundary During Institutional Control Period (mrem/year)[a]	Receptor Dose 100-m from RH-LLW Facility After Institutional Control Period (mrem/year)[b]
C-14	1.5E-03	6.1E-02
H-3	3.3E-05	7.4E-07
I-129	2.0E-05	4.9E-03
Total	1.5E-03	6.6E-02

a. Maximum dose occurs in year 2068, the first year after closure.

b. Maximum dose occurs in year 2168, 100 years after closure.

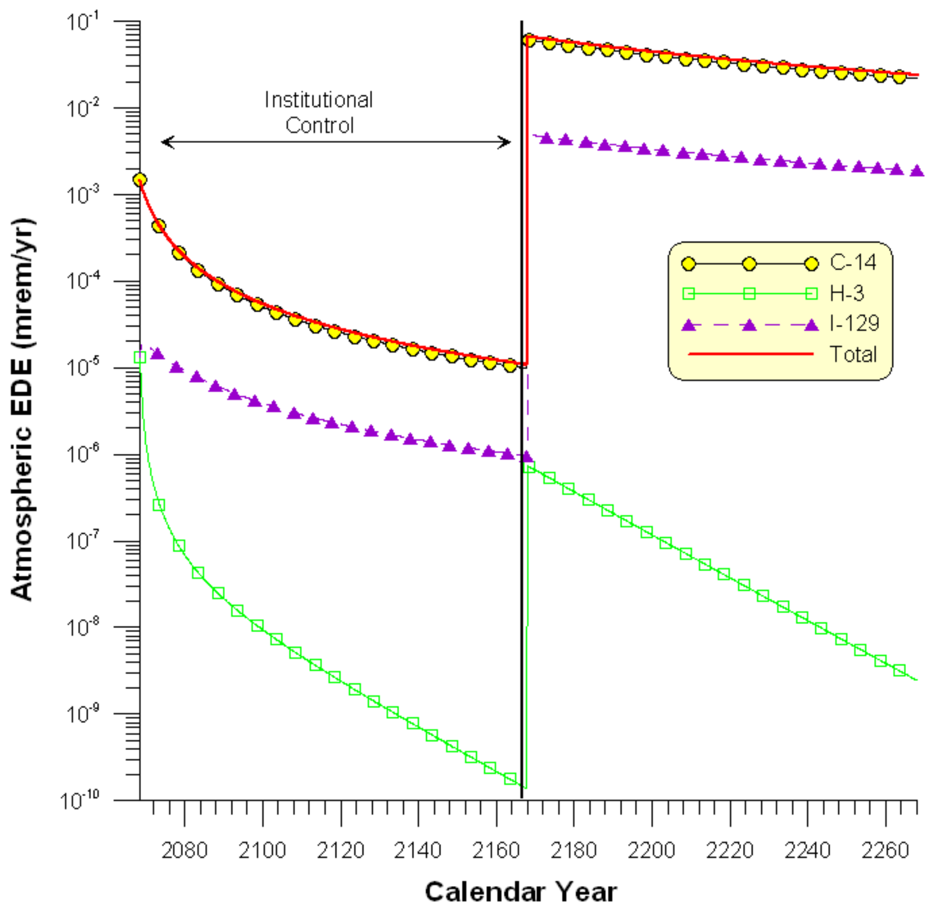

Figure 3. Air pathway dose as a function of calendar year. The dose during the institutional control period is for a receptor at the site boundary. After the institutional control period, the dose is calculated for a receptor 100-m downgradient from the disposal facility boundary.

Radon Analysis using RESRAD

Radionuclides in the projected RH-LLW inventory that are potential sources of radon include Pu-242, Ra-226, Th-230, U-234, and U-238. The only naturally occurring radionuclide in the list is Ra-226. Ra-226 concentrations in the RH-LLW disposal facility (3.05E-09 pCi/g, see Table 10) are well below background concentrations found in INL Site soils (0.75 to 1.4 pCi/g), assuming secular equilibrium with Th-230 (Rood et al. 1996).

The RESRAD computer code (Yu et al. 2001) was used to estimate the surface flux of radon from the RH-LLW inventory. RESRAD was used because it includes a radon pathway suitable for buried waste and has been used widely by the U.S. Department of Energy for deriving limits for radionuclides in soil. RESRAD tracks ingrowth of radioactive progeny and includes the progeny in the dose calculations. However, for this analysis, it is only necessary to estimate flux from the ground surface.

RESRAD uses a generalized radon pathway model to estimate the amount of radon released from the initial time of consideration. The effects of cover materials and other major parameters (e.g., geological and meteorological conditions, decay and ingrowth, and leaching and erosion) are considered with respect to near-term radon releases and long-term releases extending for thousands of years (Yu et al. 2001).

As described in the RESRAD user's manual (Yu et al. 2001), when soil is assumed to be horizontally infinite and homogeneous and the convective flow of the soil gas in the porous matrix of the soil is neglected, the radon flux J (the amount of radon activity crossing a unit area of soil surface per unit of time, Bq/[$m^2 \times s$] [pCi/($m^2 \times s$)]) can be mathematically related to the gradient of the radon concentration in the pore space, *C*, by the Fickian diffusion equation

$$J = p_t D \frac{dC}{dz} \tag{16}$$

where

p_t = total porosity

D = diffusion coefficient of radon in soil (m^2/s)

C = radon concentration in the pore space (Bq/m^3 or pCi/m^3)

z = axial distance in the direction of diffusion (m).

The radon concentration and flux along a one-dimensional direction within multiple layers of radium-contaminated soil, the cover material, and the foundation of a building are calculated by using the one-dimensional radon diffusion equation

$$\frac{d(p_t C)}{dt} = -\frac{d}{dz}(J) - p_t \lambda C + p_t Q \tag{17}$$

or

$$\frac{dC}{dt} = \frac{d}{dz}\left(D\frac{dC}{dz}\right) - \lambda C + Q \tag{18}$$

where

t = time (s)

λ = radon decay constant (1/s)

Q = radon source term into the pore space (Bq/[m^3-s] or pCi/[m^3- s]).

When steady-state conditions are assumed, Equation (17) can be written as

$$-\frac{d}{dz}\left(D\frac{dC}{dz}\right)+\lambda C=Q \tag{19}$$

The rate of radon generation, Q, or the source of radon released into the pore volume of the porous medium, is dependent on the concentration of radium in the contaminated zone. It can be evaluated by the following expression:

$$Q=\frac{\varepsilon\rho_b S_{Ra}\lambda}{p_t} \tag{20}$$

where

ε = radon emanation coefficient (dimensionless)

ρ_b = bulk density of the soil material (kg/m^3)

S_{Ra} = radium concentration in soil (Bq/kg or pCi/kg)

λ = radon decay constant (1/s).

The radon emanation coefficient, ε, represents the fraction of radon generated by radium decay that escapes from the soil particles. Radon enters air-filled pores in the soil primarily from the recoil of radon atoms during radium decay. The contribution from diffusion through the solid mineral grains is less important because most of the radon atoms decay before escaping. Observed values of ε range from about 0.01 to 0.80 (Mueller 1986). The observed emanation coefficient depends on many factors, including mineral composition of the soil, porosity, particle size distribution, and moisture content.

The radium concentration in soil, S_{Ra}, is the radon precursor principal radionuclide concentration in the contaminated soil. Its value depends on the specific radon isotope being considered. For Rn-222 or Rn-220, respectively, S_{Ra} represents the Ra-226 or Th-228 concentration in soil. The immediate parent of Rn-220 is Ra-224, which is an associated radionuclide assumed to be in equilibrium with its principal parent radionuclide Th-228.

The total porosity, or void fraction, p_t, is the fraction of the total volume that is not occupied by solid soil particles.

The boundary conditions used in RESRAD for solving Equation (19) are as follows:

$C(z_a) = 0$, the radon concentration at either the air-ground or the floor-indoor air interfaces, z_a, is zero

$J(0) = 0$, the radon flux is zero at the bottom of the boundary

$C(z)$ and $J(z)$, that is, the radon concentration and flux, respectively, are continuous across medium interfaces in the ground.

In RESRAD, Equations (16) and (19), together with the above boundary conditions, are solved numerically for the vertical profiles of C and J by using a finite-difference method. The radon flux, J, is then evaluated [from Equation (16)] at two distinct locations: (1) J_o, the outdoor flux at the interface between the ground surface and the atmosphere, and (2) J_i, the indoor flux at the interface between the floor and the indoor air.

In estimating the radon flux, the choice of a value for the diffusion coefficient, D, is critical. Values of D have been measured experimentally for a variety of materials (Nazaroff and Nero 1988; Rogers and Nielson 1991). Some of the typical values of D for different soils and building materials are summarized in the RESRAD Data Collection Handbook (Yu et al. 1993). Because the moisture content has such a dominant effect on D (i.e., much smaller effects on D are from other soil properties), D has been correlated with moisture content as (Rogers and Nielson 1991)

$$D = \left(1.1 \times 10^{-5}\right) p_t \exp\left(-6 R_s p_t - 6 R_s^{14 p_t}\right) \tag{21}$$

where

1.1×10^{-5} = the radon diffusion coefficient in free air (m^2/s)

R_s = the saturation ratio, defined as the ratio of water content over the total porosity.

This correlation is based primarily on laboratory data for earthen materials and is used in RESRAD as a default approach for the diffusion coefficient if no measured data are available for the site of interest. Nevertheless, whenever possible, site-specific diffusion coefficients should be obtained, especially for materials other than soil (Yu et al. 2001).

Parameters used to estimate the radon flux included INL site-specific data shown in Table 9. No credit was taken for any engineered features that may be used in the final cover other than 1 m of soil cover. No credit was assumed for containers or for release from activated metals. Rather the entire inventory was used to calculate the waste concentration (Table 10). All other input parameters were assigned RESRAD default values.

Table 9. Parameters used in the radon flux calculations.

Parameter	Value	Source/Comments
Waste area	2,400 m^2	Based on estimated approximate facility dimensions (240 m × 10 m) (INL 2011a)
Waste thickness	6 m	Based on two-vault stacking (INL 2011c)
Waste volume	14,400 m^3	Waste area × thickness (2,400 m^2 × 6 m)
Cover thickness	1 m	Thickness of the uppermost soil layer in the proposed ICDF cover design (EDF-9917)
Total porosity of waste zone and soil cover	0.32	Based on the properties of the uppermost soil layer in the proposed ICDF cover design (EDF-9917)
Waste zone and soil cover density	1.82 g/cm^3	Based on the properties of the uppermost soil layer in the proposed ICDF cover design (EDF-9917)
Volumetric water content of waste zone and soil cover	0.073	Based on the properties of the uppermost soil layer in the proposed ICDF cover design (EDF-9917) and an infiltration rate of 1 cm/year

Table 10. Waste concentrations used in the radon flux calculations.

Parent Radionuclide	Total Inventory (Ci)	Waste Concentration[a] (pCi/g)
Pu-242	4.00E-04	1.53E-02
Ra-226	8.00E-11	3.05E-09
Th-230	6.82E-08	2.60E-06
U-234	1.20E-03	4.58E-02
U-238	16.2	618

a. Concentration based on a bulk density of 1.82 g/cm^3 and waste volume of 14,400 m^3 (Table 9).

Screening Level Radon Flux Results

Screening level radon flux results from RESRAD are shown in Table 11. Of the radionuclides disposed of in the facility, the major contribution comes from U-238. A conservative peak total radon flux during the 1,000-year compliance period is estimated to be 3.3E-04 pCi/m^2/s which is well below the 40 CFR 61, Subpart Q standard of 20 pCi/m^2/s. Although it is beyond the 1,000-year compliance period, the 10,000-year flux results are shown in Table 11 and the total (5.9E-02 pCi/m^2/s) is still much less than the standard. Figure 4 shows that even though the radon flux continues to increase with time (due to ingrowth of progeny), the flux is approaching a steady value.

Table 11. Radon flux results (pCi/m^2/s).

Time (years from closure)	Parent Radionuclide					Total
	Pu-242	Ra-226	Th-230	U-234	U-238	
1	3.7E-28	1.0E-09	3.8E-10	3.0E-11	3.8E-13	1.4E-09
100	3.6E-20	9.8E-10	3.7E-08	2.9E-07	3.7E-07	6.9E-07
300	2.8E-18	8.8E-10	1.0E-07	2.5E-06	9.6E-06	1.2E-05
500	2.1E-17	7.9E-10	1.6E-07	6.6E-06	4.3E-05	5.0E-05
1,000	3.1E-16	6.0E-10	2.9E-07	2.4E-05	3.1E-04	3.3E-04
10,000	8.1E-13	4.3E-12	6.3E-07	4.6E-04	5.8E-02	5.9E-02

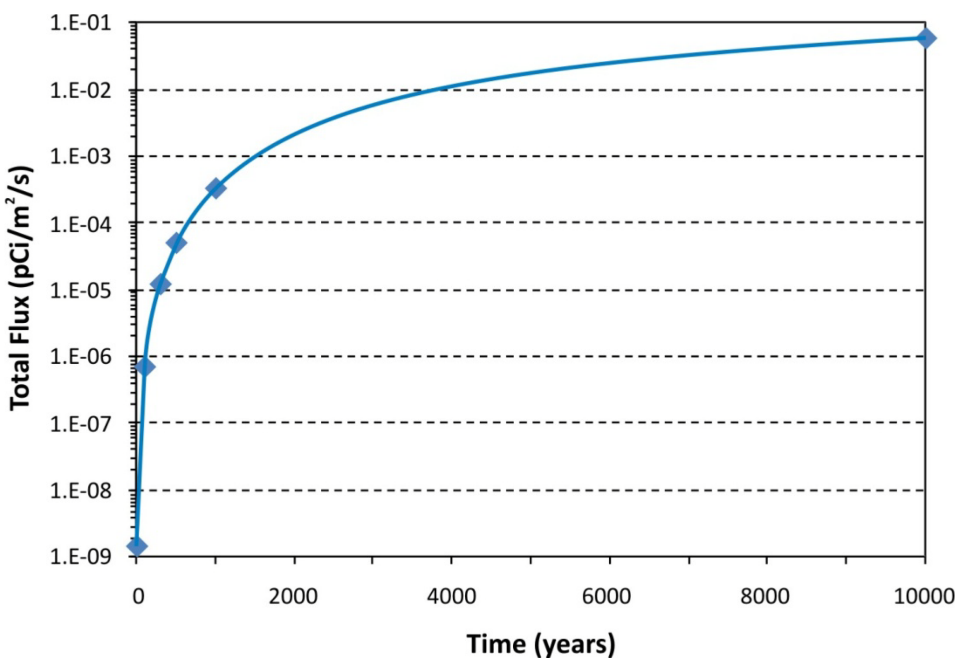

Figure 4. Calculated total radon flux after closure.

CONCLUSIONS

Based on the results of this assessment, air pathway doses from the proposed RH-LLW disposal facility are expected to be much less than the allowable standard in 40 CFR 61, Subpart H. Radon fluxes are also expected to be much less than the allowable standard in 40 CFR 61, Subpart Q.

PROJECT ENGINEER STAMP

NA

REFERENCES

40 CFR 61, Subpart H, 2006, "National Emission Standards for Emissions of Radionuclides Other than Radon from Department of Energy Facilities," *Code of Federal Regulations*, Office of the Federal Register, 2006.

40 CFR 61, Subpart Q, 2006, "National Emission Standards for Radon Emissions from Department of Energy Facilities," *Code of Federal Regulations*, Office of the Federal Register, 2006.

Cecil, L. D., J. R. Pittman, T. M. Beasley, R. L. Michel, P. W. Kubik, P. Sharma, U. Fehn, and H. Gove, 1992, "Water Infiltration Rates in the Unsaturated Zone at the Idaho National Engineering Laboratory Estimated from Chlorine-36 and Tritium Profiles, and Neutron Logging," *Proceedings of the 7th International Symposium on Water-Rock Interaction*, *Park City, Utah,* WRI-7, Rotterdam: Balkema.

Denham, M. 2010, *Vapor-Aqueous Solution Partition Coefficients for Radionuclides Pertinent to High Level Waste Tank Closure*, SRNL-TR-2010-00096, Savannah River National Laboratory, 2010.

Denham, M., D. Kaplan, and C. Yeager, 2009, *Groundwater Radioiodine: Prevalence, Biogeochemistry, and Potential Remedial Approaches*, SRNL-STI-2009-00463, Savannah River National Laboratory, September 2009.

DOE-ID, 2010, *National Emission Standards for Hazardous Air Pollutants—Calendar Year 2009 INL Report for Radionuclides*, DOE/ID-10890(10), U.S. Department of Energy Idaho Operations Office, June 2010.

DOE-ID, 2011, *Performance Assessment for the Idaho National Laboratory Remote-Handled Low-Level Waste Disposal Facility (DRAFT)*, DOE/ID-11421, U.S. Department of Energy Idaho Operations Office, November 2011.

DOE Manual 435.1-1, Change 1, 2001, "Radioactive Waste Management Manual," U.S. Department of Energy.

ECAR-851, 2010, "Estimate of the Radionuclide Content of Future Resins Generation at ATR from 2016 to 2065," Engineering Calculation and Analysis Report, Idaho National Laboratory, May 2010.

ECAR-854, 2010, "Estimate of the Radionuclide Content of Future Activated Metal Generation at ATR from 2016 to 2065," Engineering Calculation and Analysis Report, Idaho National Laboratory, January 2010.

ECAR-904, 2010, "A Methodology for Retrofitting Source-Terms to Previously Inadequately Characterized EBR-II Irradiated Reactor Hardware as Waste (Source Term and Volume Estimate for MFC Generated Remote Handled Low Level Waste from 2016 to 2065)," Engineering Calculation and Analysis Report, Idaho National Laboratory, June 2010.

ECAR-967, 2010, "Source Term and Volume Estimate for MFC Generated Remote Handled Low Level Waste from 2016 to 2065," Engineering Calculation and Analysis Report, Idaho National Laboratory, June 2010.

ECAR-1588, 2011, "RWSF Legacy Recasting Waste U and Pu Adjustments," Engineering Calculation and Analysis Report, Idaho National Laboratory, July 2011.

EDF-9917, 2011, "Atmospheric Pathway Analysis for the Idaho CERCLA Disposal Facility Landfill Performance Assessment," Idaho Cleanup Project, Idaho Falls, Idaho, February 2011.

EPA, 1997, "EMSOFT User's Guide," NCEA-W-0073, U.S. Environmental Protection Agency, February 1997 (available at: http://cfpub.epa.gov/ncea/cfm/recordisplay.cfm?deid=12461, web page updated October 4, 2010, Web page visited February 7, 2011.

EPA, 2007, "Updated User's Guide for CAP88-PC Version 3.0," EPA 402-R-00-004, U.S. Environmental Protection Agency, December 2007 (available at http://www.epa.gov/radiation/assessment/CAP88/index.html, web page updated February 2009, Web site visited November 30, 2009).

EPA, 2010, EPA On-line Tools for Site Assessment Calculation, http://www.epa.gov/athens/learn2model/part-two/onsite/estdiffusion-ext.html, web page updated October 11, 2010, Web page visited December 16, 2010.

Fox, D. T., M. A. Plummer, L. C. Hull, and D. C. Cooper, 2004, *Multiphase Carbon-14 Transport in a Near-Field-Scale Unsaturated Column of Natural Sediments*, INEEL/EXT-04-01793, Idaho National Engineering and Environmental Laboratory.

Harvego, L., J. Connolly, L. Peterson, B. Orr, and B. Starr, 2010, *Siting Study for the Remote-Handled Low-Level Waste Disposal Facility*, INL/EXT-07-12902, Idaho National Laboratory, January 2010.

INL, 2011a, *Evaluation of Groundwater Impacts to Support the National Environmental Policy Act Environmental Assessment for the INL Remote-Handled Low-Level Waste Disposal Project*, INL/EXT-10-19168, Revision 2, Idaho National Laboratory.

INL, 2011b, *Assessment of Geochemical Environment for the Proposed INL Remote Handled Low Level Waste Disposal Facility (Draft)*, INL/EXT-10-19385, Idaho National Laboratory.

INL, 2011c, *Conceptual Design Report for the Remote-Handled Low-Level Waste Disposal Facility*, INL/EXT-07-12901, Idaho National Laboratory.

Koeppen, L. D., M. D. McKenzie, P. D. Ritter, and W. A. Smith, 2006, *Fiscal Year 2005 Environmental Monitoring Report for the Radioactive Waste Management Complex*, RPT-171, Idaho Cleanup Project, Idaho National Laboratory, June 2006.

Mueller, 1986, *Indoor Air Quality Environmental Information Handbook: Radon*, DOE/PE/72013-2, Mueller Associates, Inc., January 1986.

Nazaroff, W. W. and A. V. Nero (eds.), 1988, *Radon and Its Decay Products in Indoor Air*, New York: John Wiley & Sons.

NRF, 2011, *Updated Long Range Radioactivity Estimate for NRF RH-LLW*, DRAFT Letter Report NRF-WS-603 from Noah Rupp, Naval Reactors Facility, Bechtel Marine Propulsion Corporation, Bettis Atomic Power Laboratory, to Naval Reactors Operations Manager, U.S. Department of Energy, Idaho Branch Office, April 11, 2011.

Rogers, V. C. and K. K. Nielson, 1991, "Correlations for Predicting Air Permeabilities and Rn-222 Diffusion Coefficients of Soils," *Health Physics* 61:225–230.

Rood, S. M., G. A. Harris, and G. J. White, 1996, *Background Dose Equivalent Rates and Surficial Soil Metal and Radionuclide Concentrations for the Idaho National Engineering Laboratory*, INEL-94/0250, Idaho National Engineering Laboratory.

Sander, R., 2010, Henry's Law Constants (Solubilities). http://www.mpch-mainz.mpg.de/~sander/res/henry.html, Max Planck Institute of Chemistry, Mainz, Germany, web page updated November 25, 2010, Web page visited December 16, 2010.

Yu, C., A. J. Zielen, J. J. Cheng, D. J. LePoire, E. Gnanapragasam, S. Kamboj, J. Arnish, A. Wallo III, W. A. Williams, and H. Peterson, 2001, *User's Manual for RESRAD Version 6*, ANL/EAD-4, Environmental Assessment Division, Argonne National Laboratory, July 2001.

Yu, C., C. Loureiro, J.-J. Cheng, L. G. Jones, Y. Y. Wang, Y. P. Chia, and E. Faillance, 1993, *Data Collection Handbook to Support Modeling the Impacts of Radioactive Material in Soil*, ANL/EAIS-8, Argonne National Laboratory, April 1993.

APPENDIXES

Appendix A, CAP88-PC Input Files

Appendix B, EMSOFT Source Code and Benchmark Problem Results

Appendix C, EMSOFT Input Files (Console Version) for the RH-LLW Air Pathway Analysis

Appendix D, RESRAD Input File

Appendix E, Microsoft Excel Worksheets

Appendix A, CAP88-PC Input Files

Ar39A.dat (Ar-39 Site Boundary Receptor)

```
08/02/19 1:34:00 PM           Feb  19, 2008  01:41 pm
RUN                           RUN.
C:\projects\fy2010\RHLLWPA\Atmospheric\Cfa10y.wnd

INL
PO Box 1625

Idaho Falls                  ID            83415
                                                   2008
RHLLW
Receptors 1-20
100.0000,500.0000
         0         0         0         0         0        20
     17421     18388     18786     19172     19192     20266     21330     21866
     22547     22957     24005     26561     30222     43493     43736     44016
     44439     45239     45899     45957
       800    280.20     20.80      3.54
         0         0
         1
      1.00      1.00 0.000E+00 0.000E+00
 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
         1         0         0
Ar-39              G         0 0.000e+00 0.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
        unspecified 0.000E+00 0.000E+00 0.000E+00 0.000E+00 7.053E-06
      0.70      0.30      0.00     Rural
      0.40      0.60      0.00
      0.44      0.56      0.00
F         F         T         T
 7.190e-02 8.560e-03 7.150e-02
Ar-39             18         0
        00        00        00        00        00        00
 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00
 1
Ar-39              G         0 0.000e+00 0.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 4.606E-01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
        unspecified 0.000E+00 0.000E+00 0.000E+00 0.000E+00 7.053E-06
--DecayStep--1
--LimitChildren--1
--Children--5
```

Ar39D.dat (Ar-39 100-m Receptor)

```
08/02/19 1:40:00 PM           Feb  19, 2008  01:42 pm
RUN                           RUN.
C:\projects\fy2010\RHLLWPA\Atmospheric\Cfa10y.wnd

INL
PO Box 1625

Idaho Falls                  ID            83415
                                                   2008
RHLLW
Receptors 60-62
100.0000,500.0000
         0         0         3         0         0         1
       100         0         0         0         0         0         0         0
         0         0         0         0         0         0         0         0
         0         0         0         0
       800    280.20     20.80      3.54
         0         0
         1
      1.00      1.00 0.000E+00 0.000E+00
 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
         1         0         0
Ar-39              G         0 0.000e+00 0.000e+00 5.480e-05         0
```

```
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
        unspecified 0.000E+00 0.000E+00 0.000E+00 0.000E+00 7.053E-06
      0.70      0.30      0.00     Rural
      0.40      0.60      0.00
      0.44      0.56      0.00
F         F         T         T
 7.190e-02 8.560e-03 7.150e-02
Ar-39             18         0
       00        00        00        00        00        00
 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00
 1
Ar-39              G         0 0.000e+00 0.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 4.606E-01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
        unspecified 0.000E+00 0.000E+00 0.000E+00 0.000E+00 7.053E-06
--DecayStep--1
--LimitChildren--1
--Children--5
```

C14A.dat (C-14 Site Boundary Receptor)

```
08/02/18 11:45:00 AM          Feb  18, 2008  11:49 am
RUN                           RUN.
C:\projects\fy2010\RHLLWPA\Atmospheric\Cfa10y.wnd

INL
PO Box 1625

Idaho Falls                  ID            83415
                                               2008
RHLLW
Receptors 1-20
100.0000,500.0000
         0         0         0         0         0        20
     17421     18388     18786     19172     19192     20266     21330     21866
     22547     22957     24005     26561     30222     43493     43736     44016
     44439     45239     45899     45957
       800    280.20     20.80      3.54
         0         0
         1
      1.00      1.00 0.000E+00 0.000E+00
 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
         1         0         0
C-14               G         0 1.000e+00 1.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
            dioxide 0.000E+00 0.000E+00 0.000E+00 0.000E+00 3.311E-07
      0.08      0.92      0.00     Rural
      0.00      1.00      0.00
      0.01      0.99      0.00
F         F         T         T
 7.190e-02 8.560e-03 7.150e-02
C-14               6         0
       00        00        00        00        00        00
 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00
 1
C-14               G         0 1.000e+00 1.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 4.610E-01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
            dioxide 0.000E+00 0.000E+00 0.000E+00 0.000E+00 3.311E-07
--DecayStep--1
--LimitChildren--1
--Children--5
```

C14D.dat (C-14 100-m Receptor)

```
08/02/18 11:49:00 AM          Feb  18, 2008  11:50 am
RUN                           RUN.
C:\projects\fy2010\RHLLWPA\Atmospheric\Cfa10y.wnd

INL
```

```
PO Box 1625

Idaho Falls                ID           83415
                                            2008
RHLLW
Receptors 60-62
100.0000,500.0000
         0         0         3         0         0         1
       100         0         0         0         0         0         0         0
         0         0         0         0         0         0         0         0
         0         0         0         0
       800    280.20     20.80      3.54
         0         0
         1
      1.00      1.00 0.000E+00 0.000E+00
 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
         1         0         0
C-14             G           0 1.000e+00 1.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
           dioxide 0.000E+00 0.000E+00 0.000E+00 0.000E+00 3.311E-07
      0.08      0.92      0.00     Rural
      0.00      1.00      0.00
      0.01      0.99      0.00
F        F        T        T
 7.190e-02 8.560e-03 7.150e-02
C-14             6         0
        00        00        00        00        00        00
 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00
 1
C-14             G           0 1.000e+00 1.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 4.610E-01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
           dioxide 0.000E+00 0.000E+00 0.000E+00 0.000E+00 3.311E-07
--DecayStep--1
--LimitChildren--1
--Children--5
```

H3A.dat (H-3 Site Boundary Receptor)

```
08/02/18 11:45:00 AM          Feb  18, 2008  11:49 am
RUN                           RUN.
C:\projects\fy2010\RHLLWPA\Atmospheric\Cfa10y.wnd

INL
PO Box 1625

Idaho Falls                ID           83415
                                            2008
RHLLW
Receptors 1-20
100.0000,500.0000
         0         0         0         0         0        20
     17421     18388     18786     19172     19192     20266     21330     21866
     22547     22957     24005     26561     30222     43493     43736     44016
     44439     45239     45899     45957
       800    280.20     20.80      3.54
         0         0
         1
      1.00      1.00 0.000E+00 0.000E+00
 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
         1         0         0
H-3              V           0 1.000e+00 1.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
             vapor 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.536E-04
      0.70      0.30      0.00     Rural
      0.40      0.60      0.00
      0.44      0.56      0.00
T        T        T        T
 2.030e-01 4.560e-02 1.700e-02
H-3              1         0
        00        00        00        00        00        00
 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00
 1
```

```
H-3               V         0 1.000e+00 1.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 4.534E-01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
               vapor 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.536E-04
--DecayStep--1
--LimitChildren--1
--Children--5
```

H3D.dat (H-3 100-m Receptor)

```
08/02/18 11:49:00 AM          Feb  18, 2008  11:50 am
RUN                           RUN.
C:\projects\fy2010\RHLLWPA\Atmospheric\Cfa10y.wnd

INL
PO Box 1625

Idaho Falls                 ID           83415
                                             2008
RHLLW
Receptors 60-62
100.0000,500.0000
         0         0         0         0         0         1
       100         0         0         0         0         0         0         0
         0         0         0         0         0         0         0         0
         0         0         0         0
       800    280.20     20.80      3.54
         0         0
         1
      1.00      1.00 0.000E+00 0.000E+00
 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
         1         0         0
H-3               V         0 1.000e+00 1.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
               vapor 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.536E-04
      0.70      0.30      0.00     Rural
      0.40      0.60      0.00
      0.44      0.56      0.00
T         T         T         T
 2.030e-01 4.560e-02 1.700e-02
H-3               1         0
        00        00        00        00        00        00
 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00
 1
H-3               V         0 1.000e+00 1.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 4.534E-01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
               vapor 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.536E-04
--DecayStep--1
--LimitChildren--1
--Children--5
```

I129A.dat (I-129 Site Boundary Receptor)

```
08/02/18 11:45:00 AM          Feb  18, 2008  11:49 am
RUN                           RUN.
C:\projects\fy2010\RHLLWPA\Atmospheric\Cfa10y.wnd

INL
PO Box 1625

Idaho Falls                 ID           83415
                                             2008
RHLLW
Receptors 1-20
100.0000,500.0000
         0         0         0         0         0        20
     17421     18388     18786     19172     19192     20266     21330     21866
     22547     22957     24005     26561     30222     43493     43736     44016
     44439     45239     45899     45957
       800    280.20     20.80      3.54
```

```
         0         0
         1
      1.00      1.00 0.000E+00 0.000E+00
 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
         1         0         0
I-129             V         0 1.000e+00 1.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
               vapor 2.000E-02 1.000E-01 1.000E-02 4.000E-02 1.208E-10
      0.70      0.30      0.00     Rural
      0.40      0.60      0.00
      0.44      0.56      0.00
F         F         T         T
 7.190e-02 8.560e-03 7.150e-02
I-129            53         0
        00        00        00        00        00        00
 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00
 1
I-129             V         0 1.000e+00 1.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 4.610E-01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
               vapor 2.000E-02 1.000E-01 1.000E-02 4.000E-02 1.208E-10
--DecayStep--1
--LimitChildren--1
--Children--5
```

I129D.dat (I-129 100-m Receptor)

```
08/02/18 11:49:00 AM          Feb  18, 2008  11:50 am
RUN                           RUN.
C:\projects\fy2010\RHLLWPA\Atmospheric\Cfa10y.wnd

INL
PO Box 1625

Idaho Falls                 ID            83415
                                             2008
RHLLW
Receptors 60-62
100.0000,500.0000
         0         0         0         0         0         1
       100         0         0         0         0         0         0         0
         0         0         0         0         0         0         0         0
         0         0         0         0
       800    280.20     20.80      3.54
         0         0
         1
      1.00      1.00 0.000E+00 0.000E+00
 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
         1         0         0
I-129             V         0 1.000e+00 1.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
               vapor 2.000E-02 1.000E-01 1.000E-02 4.000E-02 1.208E-10
      0.70      0.30      0.00     Rural
      0.40      0.60      0.00
      0.44      0.56      0.00
F         F         T         T
 7.190e-02 8.560e-03 7.150e-02
I-129            53         0
        00        00        00        00        00        00
 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00
 1
I-129             V         0 1.000e+00 1.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 4.610E-01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
               vapor 2.000E-02 1.000E-01 1.000E-02 4.000E-02 1.208E-10
--DecayStep--1
--LimitChildren--1
--Children--5
```

Kr81A.dat (Kr-81 Site Boundary Receptor)

```
08/02/19 1:34:00 PM           Feb  19, 2008  01:41 pm
RUN                           RUN.
C:\projects\fy2010\RHLLWPA\Atmospheric\Cfa10y.wnd

INL
PO Box 1625

Idaho Falls                  ID            83415
                                                2008
RHLLW
Receptors 1-20
100.0000,500.0000
         0         0         0         0         0        20
     17421     18388     18786     19172     19192     20266     21330     21866
     22547     22957     24005     26561     30222     43493     43736     44016
     44439     45239     45899     45957
       800    280.20     20.80      3.54
         0         0
         1
      1.00      1.00 0.000E+00 0.000E+00
 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
         1         0         0
Kr-81             G         0 0.000e+00 0.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
         unspecified 0.000E+00 0.000E+00 0.000E+00 0.000E+00 9.035E-09
      0.08      0.92      0.00     Urban
      0.00      1.00      0.00
      0.01      0.99      0.00
F         F         T         T
 7.190e-02 8.560e-03 7.150e-02
Kr-81            36         0
        00        00        00        00        00        00
 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00
 1
Kr-81             G         0 0.000e+00 0.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 4.610E-01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
         unspecified 0.000E+00 0.000E+00 0.000E+00 0.000E+00 9.035E-09
--DecayStep--1
--LimitChildren--1
--Children--5
```

Kr81D.dat (Kr-81 100-m Receptor)

```
08/02/19 1:40:00 PM           Feb  19, 2008  01:42 pm
RUN                           RUN.
C:\projects\fy2010\RHLLWPA\Atmospheric\Cfa10y.wnd

INL
PO Box 1625

Idaho Falls                  ID            83415
                                                2008
RHLLW
Receptors 60-62
100.0000,500.0000
         0         0         3         0         0         1
       100         0         0         0         0         0         0         0
         0         0         0         0         0         0         0         0
         0         0         0         0
       800    280.20     20.80      3.54
         0         0
         1
      1.00      1.00 0.000E+00 0.000E+00
 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
         1         0         0
Kr-81             G         0 0.000e+00 0.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
         unspecified 0.000E+00 0.000E+00 0.000E+00 0.000E+00 9.035E-09
      0.08      0.92      0.00     Urban
```

```
      0.00      1.00      0.00
      0.01      0.99      0.00
F         F         T         T
 7.190e-02 8.560e-03 7.150e-02
Kr-81             36         0
        00        00        00        00        00        00
 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00
 1
Kr-81              G         0 0.000e+00 0.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 4.610E-01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
        unspecified 0.000E+00 0.000E+00 0.000E+00 0.000E+00 9.035E-09
--DecayStep--1
--LimitChildren--1
--Children--5
```

Kr85A.dat (Kr-85 Site Boundary Receptor)

```
08/02/19 1:34:00 PM           Feb  19, 2008  01:41 pm
RUN                           RUN.
C:\projects\fy2010\RHLLWPA\Atmospheric\Cfa10y.wnd

INL
PO Box 1625

Idaho Falls                 ID           83415
                                              2008
RHLLW
Receptors 1-20
100.0000,500.0000
         0         0         0         0         0        20
     17421     18388     18786     19172     19192     20266     21330     21866
     22547     22957     24005     26561     30222     43493     43736     44016
     44439     45239     45899     45957
       800    280.20     20.80      3.54
         0         0
         1
      1.00      1.00 0.000E+00 0.000E+00
 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
         1         0         0
Kr-85              G         0 0.000e+00 0.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
        unspecified 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.770E-04
      0.70      0.30      0.00     Rural
      0.40      0.60      0.00
      0.44      0.56      0.00
T         T         T         T
 2.030e-01 4.560e-02 1.700e-02
Kr-85             36         0
        00        00        00        00        00        00
 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00
 1
Kr-85              G         0 0.000e+00 0.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 4.523E-01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
        unspecified 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.770E-04
--DecayStep--1
--LimitChildren--1
--Children--5
```

Kr85D.dat (Kr-85 100-m Receptor)

```
08/02/19 1:40:00 PM           Feb  19, 2008  01:42 pm
RUN                           RUN.
C:\projects\fy2010\RHLLWPA\Atmospheric\Cfa10y.wnd

INL
PO Box 1625

Idaho Falls                 ID           83415
                                              2008
```

```
RHLLW
Receptors 60-62
100.0000,500.0000
         0         0         3         0         0         1
       100         0         0         0         0         0         0         0
         0         0         0         0         0         0         0         0
         0         0         0         0
       800    280.20     20.80      3.54
         0         0
         1
      1.00      1.00 0.000E+00 0.000E+00
 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
         1         0         0
Kr-85               G         0 0.000e+00 0.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
         unspecified 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.770E-04
      0.70      0.30      0.00     Rural
      0.40      0.60      0.00
      0.44      0.56      0.00
T         T         T         T
 2.030e-01 4.560e-02 1.700e-02
Kr-85              36         0
        00        00        00        00        00        00
 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00
 1
Kr-85               G         0 0.000e+00 0.000e+00 5.480e-05         0
 1.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 4.523E-01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000e+00         0 0.000e+00
         unspecified 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.770E-04
--DecayStep--1
--LimitChildren--1
--Children--5
```

Cfa10y.wnd (meteorological data file for CAP88-PC)

```
   3.80884
 .0424 .0292 .0183 .0160 .0195 .0448 .1067 .1039 .0516 .0352 .0356 .0437 .0711 .1692 .1495 .0634
1.3931.2861.1951.1521.1451.2231.2431.1631.1791.1221.1661.2111.3021.4371.5121.536
2.6062.1272.0421.7991.8981.9381.8231.6001.8821.6532.0652.0952.2272.6462.8562.848
2.9152.6052.5692.6951.8412.3382.0681.8992.1552.0003.0652.8643.1113.4773.7333.588
3.7133.0162.8422.5872.4983.5723.1442.8532.5972.0982.3942.6603.2035.3475.8164.140
2.4092.1152.0981.5202.0732.3812.3892.2891.8301.6591.7301.8952.1702.7262.8192.489
1.1991.1141.1571.0361.0651.1421.2121.2331.1881.1151.1381.2101.2371.2741.2321.240
 .000 .000 .000 .000 .000 .000 .000 .000 .000 .000 .000 .000 .000 .000 .000 .000
1.9191.8001.6831.6211.6111.7211.7481.6371.6601.5751.6421.7051.8201.9632.0312.052
3.1212.8092.7702.6382.6102.5452.4832.3342.6882.5183.0182.9043.0963.2393.3213.302
3.6933.4993.4923.7002.9503.1852.8632.6933.2293.3924.0813.9734.1194.1034.2384.155
4.8253.8543.6843.6003.6354.6164.1733.8834.1843.4183.7833.7364.5756.9017.0555.362
3.0462.7582.7032.1222.8473.1873.0452.9082.5092.2432.2812.4632.8273.4073.4883.167
1.6881.5621.6281.4271.4801.6061.7061.7341.6731.5641.6001.7041.7391.7851.7321.743
 .000 .000 .000 .000 .000 .000 .000 .000 .000 .000 .000 .000 .000 .000 .000 .000
     .1732     .0605     .0730     .3379     .1238     .2316     .0000
     .2415     .0600     .0707     .2439     .1197     .2642     .0000
     .3552     .0448     .0514     .1678     .0902     .2907     .0000
     .4348     .0514     .0295     .1016     .0552     .3275     .0000
     .3687     .0487     .0436     .1364     .0974     .3051     .0000
     .2019     .0602     .0778     .3598     .1324     .1679     .0000
     .0770     .0397     .0774     .5528     .1501     .1031     .0000
     .0690     .0284     .0541     .4963     .2115     .1406     .0000
     .0911     .0331     .0450     .3494     .1932     .2882     .0000
     .1110     .0282     .0353     .1976     .1679     .4600     .0000
     .1087     .0295     .0337     .2047     .1528     .4707     .0000
     .0880     .0261     .0348     .2840     .1814     .3857     .0000
     .0566     .0276     .0412     .4302     .2273     .2171     .0000
     .0344     .0219     .0417     .6656     .1377     .0987     .0000
     .0472     .0375     .0685     .6536     .0960     .0972     .0000
     .1318     .0651     .0853     .3984     .1130     .2065     .0000
```

Appendix B, EMSOFT Source Code and Benchmark Problem Results

The EMSOFT computer code was obtained from the EPA National Center for Environmental Assessment website (http://cfpub.epa.gov/ncea/cfm/recordisplay.cfm?deid=12461). The source code, executable, and model documentation were downloaded. The EMSOFT code was designed to be run from a graphical-user interface using the old MS-DOS operating system. This was found to be difficult to work with in modern operating systems; however, fortunately, the computational portion of the code was written in FORTRAN and the source code was provided in the code distribution. Because the FORTRAN code used a simple text file interface, the graphical-user interface could be bypassed by constructing an input file with a text editor.

The EMSOFT FORTRAN code was modified to facilitate the reading of text files. The modified version of the EMSOFT code (called Console Version) was benchmarked with the original version using the sample problems included in the distribution and the results were identical. This appendix includes the modified EMSOFT source code (Console Version) and the results of the two benchmark problems. It also contains the text files used as input for each radionuclide simulated for the RH-LLW air pathway analysis (C-14, H-3, and I-129).

EMSOFT Source Code (Console Version)

```
      program EMCONSOL2
      implicit real*8(a-h,o-z)
c---------------------------------------------------------------------
c-----Screening Model (Jury et al, 1983: J. Envron. Qual. 12:558-564).
c-----Modified to consider buried chemicals at depth L1-L.
c-----C[z,t;(L1-L)]=C1(z,t;L1)-C(z,t;L)
c----------------------------------------------------------------------
C     SEPTEMBER, 1992
C
C     ABOVE CODE MODIFIED BY ENSR TO:
C     - ADDRESS MULTIPLE BURIED LAYERS BY SUPERPOSITION OF SINGLE-LAYER
C       SOLUTIONS
C     - CALCULATE AVERAGE CONC IN SURFACE SOIL LAYER
C     - CALCULATE AVERAGE SURFACE FLUX OVER USER-SPECIFIED TIME
C     - PROVIDE CONVENIENT USER INTERFACE
C       (IN GENERAL, ANYTHING IN UPPER-CASE LETTERS REPRESENTS A
C       MODIFICATION)
C     - Modified by A.S. Rood 6/30/08 to include:
C         --- readline subroutine to read input
C         --- variable number of points for output times


C----------------------------------------------------------------------
C     JUNE, 1996 (VERSION 1.3)
C
C     CODE MODIFIED BY ENVIRONMENTAL QUALITY MANAGEMENT TO MAKE MINOR
C     CORRECTIONS AND ENHANCEMENTS
C----------------------------------------------------------------------

C     THIS VERSION WAS MODIFIED FOR Improved Consol EXECUTION BY A.S. ROOD 01/02/2008
C     11/02/2010 - modified to produce output of cummulative flux vs time
C
C----------------------------------------------------------------------
C     VARIABLE DESCRIPTIONS (INCOMPLETE)
C     ---------------------
C     NAME    TYPE    DESCRIPTION
C     ------- ------- ------------------------------------------------
C     CHEM    CHAR*25 CHEMICAL NAME
C     KOC     REAL*8  ORGANIC CARBON PARTITION COEFFICIENT
C     KH      REAL*8  HENRY'S LAW CONSTANT
C     DVAIR   REAL*8  CHEMICAL DIFFUSION COEFF IN AIR
C     DLW     REAL*8  CHEMICAL DIFFUSION COEFF IN WATER
C     T12     REAL*8  CHEMICAL HALF LIFE
C     NLAY    INT     NUMBER OF SOIL LAYERS
C     ZP      REAL*8  DEPTH FOR PRINTING CONC RESULTS
C     FOC     REAL*8  SOIL FRACTION ORGANIC CARBON
C     O       REAL*8  SOIL WATER CONTENT
C     PB      REAL*8  SOIL BULK DENSITY
C     E       REAL*8  VERTICAL POREWATER FLUX
C     DBL     REAL*8  BOUNDARY LAYER THICKNESS
C     DL(I)   REAL*8  THICKNESS OF SOIL LAYER I
C     C0(I)   REAL*8  CHEMICAL CONCENTRATIONS IN SOIL LAYER I
C     TP      REAL*8  TIME FOR AVERAGING AND PRINTING FLUX AND CONC
C     AVD1    REAL*8  DEPTH FOR AVERAGING CONC RESULTS
C     DC      REAL*8  THICKNESS OF UNCONTAMINATED LAYER AT SURFACE
C     L1(I)   REAL*8  DEPTH OF TOP OF SOIL LAYER I
C     L(I)    REAL*8  DEPTH OF BOTTOM OF SOIL LAYER I
C     DT      REAL*8  TIME INTERVAL
C     IC,ICT  INT     IC OR ICT=1 FOR T<T0, IC OR ICT=2 FOR T>T0
```

```
C     II      INT     COUNTER FOR TIME VECTORS
C----------------------------------------------------------------------
      include 'params.inc'
      CHARACTER ENDH
      CHARACTER*3 BEG,HSKEY
      CHARACTER BEGX(3)
      EQUIVALENCE (BEG,BEGX)
C
      integer UPINDEX,UPINDEX2
C
      CHARACTER*80 DIRSTR
C
      CHARACTER*8 CFILEN(16),EFILEN(16),CHEMF,DATF,OUTF
      CHARACTER*80 DSTR
      CHARACTER*8 FIELD
      CHARACTER*20 OUTPUT(nvals+1),TACONC(nvals+1),DCONC(nvals+1)
      character*25 chem
      CHARACTER*12 ASFLUX,AVC
      CHARACTER*10 ASFT
      CHARACTER*9  AVDEP
      character*1 EFILE,CFILE,IFLAGC,IFLAG1,IFLAG2,IFLAG3,IFLAG4,IFLAG5
      CHARACTER*1 IFLAGD,IFLAGS
      real*8 Kd,Kh,Koc,Mu,L(10),L1(11),C0(10),DL(10),LL,LL1
      real*8 delt, cztav, conzt, tsp,t,flx(nvals+1),cumflx
      dimension vect(nvals+1),vecz(nvals+1),vecf(nvals+1),vecc(nvals+1)
      DIMENSION vf(nvals*5),vf1(nvals*5)
      DIMENSION VCZA(51),VCCA(51),CZAT(nvals+1)
      character*80 filein,fileout
      character*160 dline
      integer iline,npnts
      real*8 ctotal
C
      common/czft/c1(nvals*2),c2(nvals*2),c3(nvals*2),z1(nvals*2),
     & z2(nvals*2),z3(nvals*2),f1(nvals*2),f2(nvals*2),f3(nvals*2),
     & t1(nvals*2),t2(nvals*2),t3(nvals*2)
c
      data dt,t0/0.65,0.25/


C --- read input from file provided in commmand line - default file name is emconsol.par

      call getcl(filein)
      if(filein.eq.' ')then
        filein='emConsol.par'
      endif
      i=len(trim(filein))
      fileout=filein(1:i-3) // 'out'

      open(3,file=filein,status='old')

      iline=0
      call readline(dline,3,iline)
      READ(dline,'(A25)')CHEM

      call readline(dline,3,iline)
      READ(dline,*)KOC

      call readline(dline,3,iline)
      READ(dline,*)KH

      call readline(dline,3,iline)
      READ(dline,*)DVAIR

      call readline(dline,3,iline)
      READ(dline,*)DLW

      call readline(dline,3,iline)
      READ(dline,*)T12

      call readline(dline,3,iline)
      READ(dline,*)NLAY

      call readline(dline,3,iline)
      READ(dline,*)ZP

      call readline(dline,3,iline)
      READ(dline,*)TP,npnts

      call readline(dline,3,iline)
      READ(dline,*)AVD1

      call readline(dline,3,iline)
      READ(dline,*)FOC

      call readline(dline,3,iline)
      READ(dline,*)PHI

      call readline(dline,3,iline)
      READ(dline,*)O
```

```
      call readline(dline,3,iline)
      READ(dline,*)PB

      call readline(dline,3,iline)
      READ(dline,*)E

      call readline(dline,3,iline)
      READ(dline,*)DBL

      call readline(dline,3,iline)
      READ(dline,*)DC

      call readline(dline,3,iline)
      READ(dline,*)(DL(I),I=1,NLAY)

      call readline(dline,3,iline)
      READ(dline,*)(C0(I),I=1,NLAY)

      CLOSE(3)
C
      open(2,file=fileout,status='UNKNOWN')
C------------------------------
C !!!! BEGIN CALCULATIONS !!!! (finally)
C------------------------------

      L1(1)=DC
      DO 27 I=1,NLAY
        L1(I+1)=L1(I)+DL(I)
        L(I)=L1(I)+DL(I)
   27 CONTINUE

c---------------------------
c initialize some variables
c---------------------------
 8585 dt=tp/npnts
      Dz=Zp/50.
      nz=int(zp/dz+1.)
      A=Phi-O
      Mu=Dlog(2.D0)/T12
      Dlv=(Dvair*kh*A**3.33+Dlw*O**3.33)/Phi**2.
      kd=Foc*Koc
      Rl=Pb*Kd+O+A*Kh
      Rg=Rl/Kh
      H=Dvair/Dbl
      He=H/Rg
      De=Dlv/Rl
      Ve=E/Rl
      Ddt=Dt
      Dt=Ddt
      nt2=npnts
      do i=1,nt2
        flx(i)=0.0
      enddo

      write(*,*) 'dt=tp/10 ',dt
      write(*,*) 'Dz=Zp/50 ',Dz
      write(*,*) 'nz=int(zp/dz+1.) ',nz
      write(*,*) 'A=Phi-O ',A
      write(*,*) 'Mu=Dlog(2.D0)/T12 ', Mu
      write(*,*) 'Dlv=(Dvaair*kh*A**3.33+Dlw*O**3.33)/Phi**2. ',Dlv
      write(*,*) 'kd=Foc*Koc ',kd
      write(*,*) 'Rl=Pb*Kd+O+A*Kh ',Rl
      write(*,*) 'Rg=Rl/Kh ',Rg
      write(*,*) 'H=Dvair/Dbl ',H
      write(*,*) 'He=H/Rg ',He
      write(*,*) 'De=Dlv/R ',De
      write(*,*) 'Ve=E/Rl ',Ve
      write(*,*) 'Ddt=Dt ',Ddt
      write(*,*) 'Dt=Ddt ',Dt
      write(*,*) 'nt2=npnts ',nt2

      if (L1(1).le.0.0.and.nlay.eq.1) then
          ii=1
      else
          ii=0
      endif
      ict=2
c-----------------------------------------------------------
c-----Calculate surface flux versus time
c-----------------------------------------------------------
      call fl(nlay,nt2,ict,ii,dt,t0,L,L1,De,Ve,He,Mu,C0,vf,vf1
     1 ,vect,vecf,ilog)
c-----------------------------------------------------------
c-----Calculate Cumulative Volatilization (for t=Tp)------
c Modified 11/02/10 to calculate cummulative flux and average flux as a function of time
c-----------------------------------------------------------

      do j=1,nt2
        T=float(j-1)*dt+t0
```

```
        T11=Ve*t/Dsqrt(4.*De*t)
        O1=He*(He+Ve)/De
        H1=He*t/Dsqrt(4.*De*t)
        B1=Dsqrt(Ve*Ve/4./De+Mu)
        B2=B1*Dsqrt(De)
C

        do 4000 I=1,NLAY
          LL=L(I)
          LL1=L1(I)
          CALL CUFLUX(LL,T11,O1,H1,B1,B2,MU,VE,HE,DE,T,CFLUX1)
          IF (L1(I).LE.0.0.AND.I.EQ.1) THEN
            CFLUX2=0.
          ELSE
            CALL CUFLUX(LL1,T11,O1,H1,B1,B2,MU,VE,HE,DE,T,CFLUX2)
          ENDIF
          FLX(j)=FLX(j)+C0(I)*DABS(CFLUX2-CFLUX1)
 4000   CONTINUE
      enddo
C------------------------------------------------------------
C     Calculate soil concentrations
C     at 50 points from the surface down to a specified depth
c     at t=tp
c------------------------------------------------------------
  974 icz=1
      z0=0.0
      call fcz(tp,z0,nlay,nz,icz,dz,L,L1,De,Ve,He,Mu,C0,vecz,vecc)
C------------------------------------------------------------
C     Calculate average conc. over a specified depth (AVD1)
C     as a function of time
C------------------------------------------------------------
      dzav=avd1/50.
      NZAV=INT(AVD1/DZAV+1.)

      DO 10 I=1,NT2
        T=float(i-1)*dt+t0
        CALL FCZ(T,Z0,NLAY,NZAV,ICZ,DZAV,L,L1,DE,VE,HE,MU,C0,VCZA,VCCA)
c        CALL FCZ(T,zp,NLAY,NZAV,ICZ,DZAV,L,L1,DE,VE,HE,MU,C0,VCZA,VCCA)
        call intl(VCCA,NZAV,DZAV,CZAT1)
        CZAT(I)=CZAT1/AVD1
   10 CONTINUE
C------------------------------------------------------------
C-----Calculate AVERAGE CONCENTRATION OVER DEPTH AND TIME
C------------------------------------------------------------
      call intl(czat,nt2,dt,czav)
      cztav = czav/tp

C------------------
C END CALCULATIONS
C------------------
C ----- WRITE TO OUTPUT FILE(S)
C ----- ECHO INPUTS
      WRITE(2,*)' EMSOFT - Console Version 11-02-2010'
      WRITE(2,*)' EMSOFT INPUT PARAMETERS'
      WRITE(2,*)' -----------------------'
      WRITE(2,101)CHEM
      WRITE(2,102)KOC
      WRITE(2,103)KH
      WRITE(2,104)DVAIR
      WRITE(2,105)DLW
      WRITE(2,106)T12
      WRITE(2,107)FOC
      WRITE(2,108)PHI
      WRITE(2,109)O
      WRITE(2,110)PB
      WRITE(2,111)E
      WRITE(2,112)DBL
      WRITE(2,113)DC
  101 FORMAT('CHEMICAL:                       ',A25)
  102 FORMAT('KOC (ML/G):                     ',1P,E12.4)
  103 FORMAT('KH (DIMENSIONLESS):             ',1P,E12.4)
  104 FORMAT('AIR DIFF COEFF (CM2/DAY):       ',1P,E12.4)
  105 FORMAT('AQU DIFF COEFF (CM2/DAY):       ',1P,E12.4)
  106 FORMAT('HALF LIFE (DAYS):               ',1P,E12.4)
  107 FORMAT('FRACTION ORG CARBON:            ',1P,E12.4)
  108 FORMAT('SOIL POROSITY:                  ',1P,E12.4)
  109 FORMAT('SOIL WATER CONTENT:             ',1P,E12.4)
  110 FORMAT('SOIL BULK DENSITY (G/CM3):      ',1P,E12.4)
  111 FORMAT('EVAP(-)/INFILT(+) RATE (CM/DAY):',1P,E12.4)
  112 FORMAT('SURFACE BOUND LAYER (CM):       ',1P,E12.4)
  113 FORMAT('CLEAN COVER THICKNESS (CM):     ',1P,E12.4)
      WRITE(2,*)'LAYER THICKNESS (CM)   CONTAM CONC (MG/KG)'
      WRITE(2,'(8X,1P,E12.4,14X,1P,E11.4)')(DL(I),C0(I),I=1,NLAY)
      WRITE(2,*)' '
      WRITE(2,*)' EMSOFT RESULTS'
      WRITE(2,*)' --------------'

c --- Effective diffusion coefficient
      write(2,'(a42,1x,1pe10.3)')
     & 'Effective Diffusion Coefficient (cm**2/d)',de
```

```
c --- Total Initial Concentration
      write(2,*) 'Initial Mass for each Layer '
      write(2,'(3(a15))') 'Layer           ','Thickness (cm) '
     & , 'Mass (mg/cm**2)  '
      do i=1,nlay
        ctotal=C0(i)*PB/1000.D0 * DL(i)
        write(2,'(i2,13x,2(1pe10.3,5x))') i,DL(i),ctotal
      enddo

C ----- AVERAGE FLUX
C
c flx is returned in units of cm-mg/kg

      avgflx=flx(nt2)/tp*PB/1000.D0

      WRITE(2,899)TP
      WRITE(2,'(1P,E12.4)')AVGFLX
  899 FORMAT('AVERAGE FLUX FOR ',1pe12.3,' DAYS')

C ----- Total Flux
      avgflx=flx(nt2)*PB/1000.D0
      write(2,898) TP
  898 FORMAT('TOTAL FLUX FOR ',1pe12.3,' DAYS')
      WRITE(2,'(1P,E12.4)') AVGFLX
C
C ----- FLUXES vs TIME
C
      write(2,*) '  TIME        FLUX         AVG FLUX     CUM FLUX'
      write(2,*) ' (DAYS)       (MG/DAY/CM2) (MG/DAY/CM2)  (MG/CM2)'

          do 890 i=1,nt2
C              volf1=10.D0**vecf(i)*PB/1000.D0

c vecf(i) is returned in units of mg-cm/kg-d
              volf1=vecf(i)*PB/1000.D0
              if(i.eq.1)then
                avgflx=flx(i)/t0*PB/1000.D0
              else
                t=vect(i)-vect(i-1)
                avgflx=abs(flx(i)-flx(i-1))/t*PB/1000.D0
              endif
              cumflx=flx(i)*PB/1000.D0
              write(2,'(4(1pe12.5,1x))')vect(i),volf1,avgflx,cumflx
 890      continue
C
C ----- AVG CONCENTRATION
C
          WRITE(2,*)' DEPTH (CM)  AVERAGE CONC (MG/KG)'
          write(2,'(1pe12.5,1P,E12.4)')AVD1,cztav
C
C ----- AVG CONCENTRATIONS vs TIME
C
          WRITE(2,*)' TIME (DAYS)  AVERAGE CONC (MG/KG)'
c          WRITE(2,*)' TIME (DAYS)  AVERAGE CONC (MG/KG) at Zp'
          DO 885 I=1,NT2
              write(2,891)VECT(I),CZAT(I)
 885      CONTINUE
C
C ----- CONCENTRATIONS vs DEPTH
C
          WRITE(2,*)' DEPTH (CM)  CONC (MG/KG)'
          do 870 i=1,nz
              write(2,891) vecz(i),vecc(i)
 870      continue

C
 891  format(2(1pe12.5,1x))


      CLOSE(2)
      end
c-----------------------------------------------------------------
c---- S U B R O U T I N E S -------------------------------------
c-----------------------------------------------------------------
c------------
c>>>> FLUX
C------------
      subroutine fl(nlay,nt,ic,ii,dt,t0,L,L1,De,Ve,He,Mu,C0,Vf,Vf1
     1 ,vect,vecf,ilog)
c-----------------------------------------------------------------
      implicit real*8(a-h,o-z)
      include 'params.inc'
      real*8 L(10),L1(11),Mu,c0(10)
      dimension vect(nvals+1),vecf(nvals+1),vf(nvals+1),vf1(nvals+1)
      DIMENSION VCZA(51),VCCA(51)
C
C INITIALIZE ARRAYS
C ----------------
      DO 1 I=1,nvals+1
```

```
         VECT(I)=0.
         VECF(I)=0.
    1 CONTINUE
      DO 2 I=1,nvals+1
         VF(I)=0.
         VF1(I)=0.
    2 CONTINUE
c--------------------
c     loop over time
c--------------------
      do 600 i=1,nt
c
c     re-initialize variables
c     -----------------------
         ilog=0
         c1temp=0.
         ctemp=0.
         flux=0.
c
c     calculate time
c     --------------
         T=float(i-1)*dt+t0
c
         D1=2.*Dsqrt(De*T)
         P1=(-Ve*T)/D1
         P4=((Ve+2.*He)*T)/D1
         call Erf(P1,X1)
         Y1=(He+Ve)*He*T/De
         call Erfc(P4,Y1,X3)
         if (P4.eq.0.0) then
             call Erf(P4,X4)
             X3=Dexp(Y1)*(1.-X4)
         endif
         Dg=Dexp(-T*Mu)
C------------------------
C  LOOP OVER SOIL LAYERS
C------------------------
         DO 500 j=1,nlay
C---------------------
c  solution for L(j)
C---------------------
             P0=(-L(j)-Ve*T)/D1
             P5=(L(j)+(2.*He+Ve)*T)/D1
             call Erf(P0,X2)
             Csm=Ve*(X1-X2)/2.
             Y2=Y1+He*L(j)/De
             call Erfc(P5,Y2,X5)
             if (P5.lt.0.0) then
                 call Erf(P5,X6)
                 X5=Dexp(Y2)*(1.-X6)
             endif
c             write(*,'(8(1pe10.3))') Csm,He,Ve,X1,X2,X3,X5,L(j)

             Csm=Csm-(2.*He+Ve)/2.*(X3-X5)
C
             ctemp=ctemp+csm*C0(J)
             vf(i)=vf(i)-Dg*Csm*C0(J)
C
C-----------------------
c  solution for L1(j)
C-----------------------------------------------------------------
C     if the first layer is not buried, and there's only one layer,
c-----------------------------------------------------------------
             IF (L1(j).eq.0.0.and.nlay.eq.1) THEN
                 Csm1=0.0
  611            vect(i)=t
C                 vecf(i)=vecf(i)+dlog10(-Dg*Csm*C0(j))
                 vecf(i)=vecf(i)+(-Dg*Csm*C0(j))

                 GO TO 600
C
             ELSE
c----------------------------------------------------------
c     otherwise, if the first layer isn't buried, then....
c----------------------------------------------------------
                 if (L1(j).eq.0.0.AND.J.EQ.1) then
                     flux=flux-csm
                     C1TEMP=0.
                     go to 500
                 endif
c----------------------------------------------------------------
c       for all other situations, go through the full calculation
c----------------------------------------------------------------
 6241            P0=(-L1(j)-Ve*T)/D1
                 P5=(L1(j)+(2.*He+Ve)*T)/D1
                 call Erf(P0,X2)
                 Csm1=Ve*(X1-X2)/2.
                 Y2=Y1+He*L1(j)/De
                 call Erfc(P5,Y2,X5)
                 if (P5.lt.0.0) then
```

```
                    call Erf(P5,X6)
                    X5=Dexp(Y2)*(1.-X6)
                endif
                Csm1=Csm1-(2.*He+Ve)/2.*(X3-X5)
                c1temp=c1temp+csm1*C0(J)
                flux=flux+(csm1-csm)
                vf1(i)=vf1(i)-Dg*Csm1
            ENDIF
  500     continue
c-------------------------------
c     end loop over soil layers
c-------------------------------
            vect(I)=t
            vecf(I)=vecf(I)+(Dg*Dabs(C1temp-Ctemp))
C
  600 continue
c------------------------
c     end loop over time
c------------------------
      return
      end
C---------------------------------------------------------------------
C---------------------------------------------------------------------
C>>>> CONCENTRATION AS A FUNCTION OF DEPTH
C---------------------------------------------------------------------
      subroutine Fcz(t,z0,nlay,nz,icz,dz,L,L1,De,Ve,He,Mu,C0,vecz,
     1 vecc)
c---------------------------------------------------------------------
      implicit real*8(a-h,o-z)
      include 'params.inc'
      real*8 L(10),L1(11),Mu,C0(10)
      dimension vecz(nvals+1),vecc(nvals+1)
C
      D1=2.*Dsqrt(De*T)
      Dg=Dexp(-T*Mu)
C
C      do 10 i=1,nvals+1
C        vecz(i)=0.
C        vecc(i)=0.
C   10 continue
c--------------------
c     loop over depth
c--------------------
      do 901 i=1,nz
          CSUM=0.0
          Z=float(i-1)*dz+z0
          P1=(Z-Ve*T)/D1
          P3=(Z+Ve*T)/D1
          P4=(Z+(Ve+2.*He)*T)/D1
          call Erf(P1,X1)
          Y1=(He+Ve)*He*T/De+Z*(He+Ve)/De
          call Erfc(P4,Y1,X3)
          if (P4.eq.0.0) then
              call Erf(P4,X4)
              X3=Dexp(Y1)*(1.-X4)
          endif
          P22=Ve*Z/De
          P33=Ve*Z/De
          call Erfc(P3,P33,X8)
          IF (P3.lt.0.) THEN
              call Erf(P3,X9)
              X8=(1.-X9)*Dexp(Ve*Z/De)
          ENDIF
c------------------------
c       loop over layers
c------------------------
c       solution for L(j)
c------------------------
          DO 900 j=1,nlay
              P0=(Z-L(j)-Ve*T)/D1
              P2=(Z+L(j)+Ve*T)/D1
              P5=(Z+L(j)+(2.*He+Ve)*T)/D1
              call Erf(P0,X2)
              Csm=(X1-X2)/2.
              Y2=Y1+He*L(j)/De
              call Erfc(P5,Y2,X5)
              if (p5.le.0.) then
                  call Erf(P5,X6)
                  X5=Dexp(Y2)*(1.-X6)
              endif
              Csm=Csm+(2.+Ve/He)/2.*(X3-X5)
              call Erfc(P2,P22,X7)
              IF (P2.lt.0.) THEN
                  call Erf(P2,X6)
                  X7=Dexp(Ve*Z/De)*(1.-X6)
              ENDIF
              Csm=Csm+(1.+Ve/He)*(X7-X8)/2.
              Csm=Csm*Dg
c----------------------------
c         solution for L1(j)
```

```
c----------------------------
              if (L1(j).gt.0.0) go to 4246
              Csm1=0.0
              go to 4249
 4246         P0=(Z-L1(j)-Ve*T)/D1
              P2=(Z+L1(j)+Ve*T)/D1
              P5=(Z+L1(j)+(2.*He+Ve)*T)/D1
              call Erf(P0,X2)
              Csm1=(X1-X2)/2.
              Y2=Y1+He*L1(j)/De
              call Erfc(P5,Y2,X5)
              if (p5.le.0.) then
                  call Erf(P5,X6)
                  X5=Dexp(Y2)*(1.-X6)
              endif
              Csm1=Csm1+(2.+Ve/He)/2.*(X3-X5)
              call Erfc(P2,P22,X7)
              IF (P2.lt.0.) THEN
                  call Erf(P2,X6)
                  X7=Dexp(Ve*Z/De)*(1.-X6)
              ENDIF
              P33=Ve*Z/De
              call Erfc(P3,P33,X8)
              IF (P3.lt.0.) THEN
                  call Erf(P3,X9)
                  X8=(1.-X9)*Dexp(Ve*Z/De)
              ENDIF
              Csm1=Csm1+(1.+Ve/He)*(X7-X8)/2.
              Dg=Dexp(-T*Mu)
              Csm1=Csm1*Dg
 4249         conc=Dabs(Csm1-Csm)*C0(j)
              if (icz.gt.1) go to 900
              CSUM=CSUM+CONC
  900     continue
c------------------------------
c       end of loop over layers
c------------------------------
          IF (ICZ.GT.1) GO TO 901
          vecC(i)=CSUM
          vecz(i)=z
  901 continue
c----------------------------
c     end of loop over depth
c----------------------------
      return
      end
C---------------------------------------------
C---------------------------------------------
C     SUBROUTINE TO CALCULATE CUMULATIVE FLUX
C---------------------------------------------
      SUBROUTINE CUFLUX(L,T1,O1,H1,B1,B2,MU,VE,HE,DE,T,FLX)
      implicit real*8(a-h,o-z)
      REAL*8 L,MU
      Flx=0.0
      P1=Ve*L/De
      X1=L/Dsqrt(4.*De*t)
      call Erfc(t1,0.0D0,s1)
      Z1=T1+X1
      call Erfc(Z1,0.0D0,s2)
C      call Erfc(t1+2.*h1,O1*t,s3)
      Z2=T1+2.*H1
      Z3=O1*T
      call Erfc(Z2,Z3,s3)
C      call Erfc(t1+x1+2.*h1,O1*t+He*L/De,s4)
      Z4=T1+X1+2.*H1
      Z5=O1*T+HE*L/DE
      call Erfc(Z4,Z5,s4)
C      call Erfc(x1-b1*t**(0.5),-p1/2.-b1*L/De**(0.5),s5)
      Z6=x1-b1*t**(0.5)
      Z7=-p1/2.-b1*L/De**(0.5)
      call Erfc(Z6,Z7,s5)
C      call Erfc(x1+b1*t**(0.5),-p1/2.+b1*L/De**(0.5),s6)
      Z8=x1+b1*t**(0.5)
      Z9=-p1/2.+b1*L/De**(0.5)
      call Erfc(Z8,Z9,s6)
C      call Erf(b1*t**(0.5),s7)
      Z10=b1*t**(0.5)
      call Erf(Z10,s7)
      Xsu1=Ve/Mu*(1.-Dexp(-Mu*t)*(s1-s2))
      Xsu2=Xsu1-(Ve+2.*He)/(Mu-O1)*(1.-Dexp(-Mu*t)*(s3-s4))
      Xsu3=Xsu2+s5*((Ve+2.*He)/(2.*(Mu-O1))-Ve/(2.*Mu)-
     1(Ve+2.*He)*(Ve+2.*He)/(4.*(Mu-O1)*b2)+Ve*Ve/(4.*Mu*b2))
      Xsu4=Xsu3+s6*((Ve+2.*He)/(2.*(Mu-O1))-Ve/(2.*Mu)+
     1(Ve+2.*He)*(Ve+2.*He)/(4.*(Mu-O1)*b2)-Ve*Ve/(4.*Mu*b2))
      Xsu5=Xsu4/2.+1./4./b2*((Ve+2.*He)*(Ve+2.*He)/(Mu-O1)-Ve*Ve/Mu)*s7
      Flx=-Xsu5
      RETURN
      END
c--------------------------------------------------------------------------
```

```
c-------------------------------------------------------------------------
c     This is the error function subroutine. Feed in A and return B=erf(A).
C-------------------------------------------------------------------------
      subroutine Erf(Arg,B)
      implicit real*8(a-h,o-z)
      Store=0.
      IF (Arg.lt.0.) THEN
          Store=Arg
          Arg=-Arg
      ENDIF
      B=1./(1.+.3275911*Arg)
      Btem=.254829592*B-.284496736*B*B+1.421413741*B*B*B
     1 -1.453152027*B*B*B*B
      IF (dabs(Arg*ARG).gt.170.) THEN
          B=1.
          GO TO 405
      ENDIF
      B=1.-(Btem+1.061405429*B**5.)*Dexp(-Arg*Arg)
  405 IF(Store.lt.0.) THEN
          B=-B
          Arg=-Arg
      ENDIF
      RETURN
      END
c--------------------------------------------------------
C SUBROUTINE TO EVALUATE THE COMPLEMENTARY ERROR FUNCTION
C--------------------------------------------------------
      subroutine Erfc(Arg,Exparg,B)
      implicit real*8(a-h,o-z)
      IF(Arg.lt.0.) THEN
          CALL Erf(Arg,B)
          B=Dexp(Exparg)*(1.-B)
          GO TO 427
      ENDIF
      IF(Arg.gt.3.5) THEN
          CALL Erfc2(Arg,Exparg,B)
          GO TO 427
      ENDIF
      B=1./(1.+.3275911*Arg)
      Btem=.254829592*B-.284496736*B*B+1.421413741*B*B*B
     1 -1.453152027*B*B*B*B
      IF(dabs(-Arg*Arg+Exparg).gt.170.) THEN
          B=0.0
          GO TO 427
      ENDIF
      B=(Btem+1.061405429*B**5.)*Dexp(-Arg*Arg+Exparg)
  427 RETURN
      END
c-------------------------------------------------------
      subroutine Erfc2(Arg,Exparg,B)
      implicit real*8(a-h,o-z)
      pi=3.141592654
      IF(dabs(-Arg*Arg+Exparg).gt.170.) THEN
          B=0.0
          RETURN
      ENDIF
      B=Dexp(-Arg*Arg+Exparg)/Dsqrt(PI)*(1./Arg-1./(2.*Arg*Arg*Arg)
     1 +3./(4.*Arg**5.))
      RETURN
      END
c--------------------------------------------------------
      subroutine intl(y,n,h,sum)
C
C     INTEGRATION ROUTINE
c--------------------------------------------------------
      implicit real*8(a-h,o-z)
      include 'params.inc'
      dimension y(nvals)
c*      n2=n-2
      n1=n-1
      nn=n/2
      nb=nn*2
      if(n.eq.nb) go to 10
c-----Trapezoidal Rule--------
   10 sums=0.0
      do 14 i=2,n1
          sums=sums+y(i)
   14 continue
      sums=h*(sums+0.5*(y(1)+y(n)))
      sum=sums
  100 return
      end

      subroutine readline(dline,iunit,iline)
c ===============================================
c Modual Name: READLINE
c Author:  A. S. Rood
c Date Created: 12/21/99
c Last Modified: 12/21/99
c               10/21/04 - Added logical to skip blank lines
```

```
c Purpose:   reads a line from the iunit file and eather discards it
c            or passes it back to the calling rountine
c Arguments:
c  dline: character*160 to hold values on line
c  warning: waraning statement on acount of an error
c  iunit: the file unit to be read from
c  iline: index number to read file

c Called By: MAIN
c Calls To: none
c ===================================================
      implicit none
      integer iunit,iline,length,i,iflag
      character*160 dline
      character*42 warning

      warning='Error in input file on line '
 10   iline=iline+1
      read(iunit,'(a160)',err=99) dline
      if(ichar(dline(1:1)).eq.36)then   ! comment line
        goto 10
      endif
      length=len(dline)
      iflag=0
      i=1
      do while (i.lt.length)
        if(ichar(dline(i:i)).ne.13.and.ichar(dline(i:i)).ne.32)then  ! if any character other than a space
          iflag=1                                                    ! or carriage return is encountered, then
          i=length
        endif                                                        ! read the line
        i=i+1
      enddo
      if(iflag.eq.0) goto 10
      write(*,*) iline,dline(1:40)
      return
 99   write(*,'(1x,a42,1x,i3)') WARNING,iline
      write(2,'(1x,a42,1x,i3)') WARNING,iline
      stop
      end
```

Comparison to Benzene Benchmark Problem Results from EMSOFT User Manual, Appendix A.

Time (days)	Benzene Surface Flux from Appendix A (mg/cm^2-d)	Benzene Surface Flux from EMCONSOL2 (mg/cm^2-d)	Benzene Average Concentration from Appendix A (mg/kg)	Benzene Average Concentration from EMCONSOL2 (mg/kg)	Depth (m)	Benzene Depth Concentration in Appendix A (mg/kg)	Benzene Depth Concentration from EMCONSOL2 (mg/kg)
0.25	9.22E+00	9.22E+00	8.18E+01	8.18E+01	0	5.43E-05	5.43E-05
109.75	2.79E-01	2.79E-01	2.53E+00	2.53E+00	0.1	1.90E-04	1.90E-04
219.25	1.25E-01	1.25E-01	1.13E+00	1.13E+00	0.2	3.25E-04	3.25E-04
328.75	7.36E-02	7.36E-02	6.68E-01	6.68E-01	0.3	4.60E-04	4.60E-04
438.25	4.98E-02	4.98E-02	4.52E-01	4.52E-01	0.4	5.96E-04	5.96E-04
547.75	3.65E-02	3.65E-02	3.31E-01	3.31E-01	0.5	7.31E-04	7.31E-04
657.25	2.82E-02	2.82E-02	2.56E-01	2.56E-01	0.6	8.66E-04	8.66E-04
766.75	2.26E-02	2.26E-02	2.05E-01	2.05E-01	0.7	1.00E-03	1.00E-03
876.25	1.87E-02	1.87E-02	1.69E-01	1.69E-01	0.8	1.14E-03	1.14E-03
985.75	1.57E-02	1.57E-02	1.43E-01	1.43E-01	0.9	1.27E-03	1.27E-03
1095.25	1.35E-02	1.35E-02	1.22E-01	1.22E-01	1	1.41E-03	1.41E-03
1204.75	1.17E-02	1.17E-02	1.06E-01	1.06E-01	1.1	1.54E-03	1.54E-03
1314.25	1.03E-02	1.03E-02	9.36E-02	9.36E-02	1.2	1.68E-03	1.68E-03
1423.75	9.16E-03	9.16E-03	8.31E-02	8.31E-02	1.3	1.81E-03	1.81E-03
1533.25	8.21E-03	8.21E-03	7.45E-02	7.45E-02	1.4	1.95E-03	1.95E-03
1642.75	7.41E-03	7.41E-03	6.72E-02	6.72E-02	1.5	2.08E-03	2.08E-03
1752.25	6.73E-03	6.73E-03	6.10E-02	6.10E-02	1.6	2.22E-03	2.22E-03
1861.75	6.14E-03	6.14E-03	5.57E-02	5.57E-02	1.7	2.36E-03	2.36E-03
1971.25	5.64E-03	5.64E-03	5.11E-02	5.11E-02	1.8	2.49E-03	2.49E-03
2080.75	5.20E-03	5.20E-03	4.71E-02	4.71E-02	1.9	2.63E-03	2.63E-03
2190.25	4.81E-03	4.81E-03	4.36E-02	4.36E-02	2	2.76E-03	2.76E-03
2299.75	4.47E-03	4.47E-03	4.05E-02	4.05E-02	2.1	2.90E-03	2.90E-03
2409.25	4.16E-03	4.16E-03	3.78E-02	3.78E-02	2.2	3.03E-03	3.03E-03
2518.75	3.89E-03	3.89E-03	3.53E-02	3.53E-02	2.3	3.17E-03	3.17E-03

Time (days)	Benzene Surface Flux from Appendix A (mg/cm^2-d)	Benzene Surface Flux from EMCONSOL2 (mg/cm^2-d)	Benzene Average Concentration from Appendix A (mg/kg)	Benzene Average Concentration from EMCONSOL2 (mg/kg)	Depth (m)	Benzene Depth Concentration in Appendix A (mg/kg)	Benzene Depth Concentration from EMCONSOL2 (mg/kg)
2628.25	3.65E-03	3.65E-03	3.31E-02	3.31E-02	2.4	3.30E-03	3.30E-03
2737.75	3.43E-03	3.43E-03	3.11E-02	3.11E-02	2.5	3.44E-03	3.44E-03
2847.25	3.23E-03	3.23E-03	2.93E-02	2.93E-02	2.6	3.57E-03	3.57E-03
2956.75	3.05E-03	3.05E-03	2.77E-02	2.77E-02	2.7	3.71E-03	3.71E-03
3066.25	2.88E-03	2.88E-03	2.62E-02	2.62E-02	2.8	3.85E-03	3.85E-03
3175.75	2.73E-03	2.73E-03	2.48E-02	2.48E-02	2.9	3.98E-03	3.98E-03
3285.25	2.59E-03	2.59E-03	2.35E-02	2.35E-02	3	4.12E-03	4.12E-03
3394.75	2.47E-03	2.47E-03	2.24E-02	2.24E-02	3.1	4.25E-03	4.25E-03
3504.25	2.35E-03	2.35E-03	2.13E-02	2.13E-02	3.2	4.39E-03	4.39E-03
3613.75	2.24E-03	2.24E-03	2.03E-02	2.03E-02	3.3	4.52E-03	4.52E-03
3723.25	2.14E-03	2.14E-03	1.94E-02	1.94E-02	3.4	4.66E-03	4.66E-03
3832.75	2.04E-03	2.04E-03	1.85E-02	1.85E-02	3.5	4.79E-03	4.79E-03
3942.25	1.96E-03	1.96E-03	1.78E-02	1.78E-02	3.6	4.93E-03	4.93E-03
4051.75	1.88E-03	1.88E-03	1.70E-02	1.70E-02	3.7	5.07E-03	5.07E-03
4161.25	1.80E-03	1.80E-03	1.63E-02	1.63E-02	3.8	5.20E-03	5.20E-03
4270.75	1.73E-03	1.73E-03	1.57E-02	1.57E-02	3.9	5.34E-03	5.34E-03
4380.25	1.66E-03	1.66E-03	1.51E-02	1.51E-02	4	5.47E-03	5.47E-03
4489.75	1.60E-03	1.60E-03	1.45E-02	1.45E-02	4.1	5.61E-03	5.61E-03
4599.25	1.54E-03	1.54E-03	1.40E-02	1.40E-02	4.2	5.74E-03	5.74E-03
4708.75	1.48E-03	1.48E-03	1.35E-02	1.35E-02	4.3	5.88E-03	5.88E-03
4818.25	1.43E-03	1.43E-03	1.30E-02	1.30E-02	4.4	6.01E-03	6.01E-03
4927.75	1.38E-03	1.38E-03	1.25E-02	1.25E-02	4.5	6.15E-03	6.15E-03
5037.25	1.33E-03	1.33E-03	1.21E-02	1.21E-02	4.6	6.29E-03	6.29E-03
5146.75	1.29E-03	1.29E-03	1.17E-02	1.17E-02	4.7	6.42E-03	6.42E-03
5256.25	1.25E-03	1.25E-03	1.13E-02	1.13E-02	4.8	6.56E-03	6.56E-03
5365.75	1.21E-03	1.21E-03	1.10E-02	1.10E-02	4.9	6.69E-03	6.69E-03
5475.25	1.17E-03	1.17E-03	1.06E-02	1.06E-02	5	6.83E-03	6.83E-03
5584.75	1.13E-03	1.13E-03	1.03E-02	1.03E-02			
5694.25	1.10E-03	1.10E-03	9.97E-03	9.97E-03			
5803.75	1.07E-03	1.07E-03	9.68E-03	9.68E-03			
5913.25	1.04E-03	1.04E-03	9.39E-03	9.39E-03			
6022.75	1.01E-03	1.01E-03	9.12E-03	9.12E-03			
6132.25	9.77E-04	9.77E-04	8.87E-03	8.87E-03			
6241.75	9.50E-04	9.50E-04	8.62E-03	8.62E-03			
6351.25	9.24E-04	9.24E-04	8.38E-03	8.38E-03			
6460.75	8.99E-04	8.99E-04	8.16E-03	8.16E-03			
6570.25	8.75E-04	8.75E-04	7.94E-03	7.94E-03			
6679.75	8.52E-04	8.52E-04	7.73E-03	7.73E-03			
6789.25	8.30E-04	8.30E-04	7.53E-03	7.53E-03			
6898.75	8.09E-04	8.09E-04	7.34E-03	7.34E-03			
7008.25	7.89E-04	7.89E-04	7.16E-03	7.16E-03			
7117.75	7.70E-04	7.70E-04	6.98E-03	6.98E-03			
7227.25	7.51E-04	7.51E-04	6.81E-03	6.81E-03			
7336.75	7.33E-04	7.33E-04	6.65E-03	6.65E-03			
7446.25	7.15E-04	7.15E-04	6.49E-03	6.49E-03			
7555.75	6.99E-04	6.99E-04	6.34E-03	6.34E-03			
7665.25	6.83E-04	6.83E-04	6.19E-03	6.19E-03			
7774.75	6.67E-04	6.67E-04	6.05E-03	6.05E-03			
7884.25	6.52E-04	6.52E-04	5.92E-03	5.92E-03			
7993.75	6.38E-04	6.38E-04	5.79E-03	5.79E-03			

Time (days)	Benzene Surface Flux from Appendix A (mg/cm^2-d)	Benzene Surface Flux from EMCONSOL2 (mg/cm^2-d)	Benzene Average Concentration from Appendix A (mg/kg)	Benzene Average Concentration from EMCONSOL2 (mg/kg)	Depth (m)	Benzene Depth Concentration in Appendix A (mg/kg)	Benzene Depth Concentration from EMCONSOL2 (mg/kg)
8103.25	6.24E-04	6.24E-04	5.66E-03	5.66E-03			
8212.75	6.10E-04	6.10E-04	5.54E-03	5.54E-03			
8322.25	5.97E-04	5.97E-04	5.42E-03	5.42E-03			
8431.75	5.85E-04	5.85E-04	5.30E-03	5.30E-03			
8541.25	5.72E-04	5.72E-04	5.19E-03	5.19E-03			
8650.75	5.60E-04	5.60E-04	5.09E-03	5.09E-03			
8760.25	5.49E-04	5.49E-04	4.98E-03	4.98E-03			
8869.75	5.38E-04	5.38E-04	4.88E-03	4.88E-03			
8979.25	5.27E-04	5.27E-04	4.78E-03	4.78E-03			
9088.75	5.17E-04	5.17E-04	4.69E-03	4.69E-03			
9198.25	5.07E-04	5.07E-04	4.60E-03	4.60E-03			
9307.75	4.97E-04	4.97E-04	4.51E-03	4.51E-03			
9417.25	4.87E-04	4.87E-04	4.42E-03	4.42E-03			
9526.75	4.78E-04	4.78E-04	4.34E-03	4.34E-03			
9636.25	4.69E-04	4.69E-04	4.26E-03	4.26E-03			
9745.75	4.60E-04	4.60E-04	4.18E-03	4.18E-03			
9855.25	4.52E-04	4.52E-04	4.10E-03	4.10E-03			
9964.75	4.44E-04	4.44E-04	4.03E-03	4.03E-03			
10074.25	4.36E-04	4.36E-04	3.95E-03	3.95E-03			
10183.75	4.28E-04	4.28E-04	3.88E-03	3.88E-03			
10293.25	4.20E-04	4.20E-04	3.82E-03	3.82E-03			
10402.75	4.13E-04	4.13E-04	3.75E-03	3.75E-03			
10512.25	4.06E-04	4.06E-04	3.68E-03	3.68E-03			
10621.75	3.99E-04	3.99E-04	3.62E-03	3.62E-03			
10731.25	3.92E-04	3.92E-04	3.56E-03	3.56E-03			
10840.75	3.86E-04	3.86E-04	3.50E-03	3.50E-03			

Benzene Benchmark Problem Input File for EMSOFT (Console Version)

```
BENZENE                                                                          READ(3,'(A25)')CHEM
  5.8900E+01     koc (mL/g)        KOC ORGANIC CARBON PARTITION COEFFICIENT        READ(3,*)KOC
  2.2800E-01     kh  (dimensionless henry's law)  HENRY'S LAW CONSTANT             READ(3,*)KH
  7.6032E+03     Dair (cm2/day)    DVAIR   CHEMICAL DIFFUSION COEFF IN AIR         READ(3,*)DVAIR
  8.4672E-01     Dwat (cm2/day)    DLW     CHEMICAL DIFFUSION COEFF IN WATER       READ(3,*)DLW
  1.0000E+06     Thalf (days)      T12     CHEMICAL HALF LIFE                      READ(3,*)T12
     1           NLAY     NUMBER OF SOIL LAYERS                                    READ(3,*)NLAY
  5.0000E+00     ZP       DEPTH FOR PRINTING CONC RESULTS                          READ(3,*)ZP
  1.0950E+04  100   TP  npnts     TIME FOR AVERAGING AND PRINTING FLUX AND CONC            READ(3,*)TP
  5.0000E+00     AVD1     DEPTH FOR AVERAGING CONC RESULTS                         READ(3,*)AVD1
  6.0000E-03     foc                                                               READ(3,*)FOC
  4.3400E-01     phi                                                               READ(3,*)PHI
  1.5000E-01     theta                                                             READ(3,*)O
  1.5000E+00     rho                                                               READ(3,*)PB
  8.2000E-02     E        VERTICAL POREWATER FLUX                                  READ(3,*)E
  5.0000E-01     surf bnd layer (cm)  DBL     BOUNDARY LAYER THICKNESS             READ(3,*)DBL
  0.0000E+00     THICKNESS OF UNCONTAMINATED LAYER AT SURFACE                      READ(3,*)DC
  3.0000E+02     (DL(I),I=1,NLAY)  THICKNESS OF SOIL LAYER I                       READ(3,*)(DL(I),I=1,NLAY)
  4.0000E+02     (C0(I),I=1,NLAY)  CHEMICAL CONCENTRATIONS IN SOIL LAYER I         READ(3,*)(C0(I),I=1,NLAY)

  EMSOFT - Console Version 11-02-2010
  EMSOFT INPUT PARAMETERS
  -----------------------
CHEMICAL:                         BENZENE
KOC (ML/G):                       5.8900E+01
KH (DIMENSIONLESS):               2.2800E-01
AIR DIFF COEFF (CM2/DAY):         7.6032E+03
AQU DIFF COEFF (CM2/DAY):         8.4672E-01
HALF LIFE (DAYS):                 1.0000E+06
FRACTION ORG CARBON:              6.0000E-03
SOIL POROSITY:                    4.3400E-01
SOIL WATER CONTENT:               1.5000E-01
SOIL BULK DENSITY (G/CM3):        1.5000E+00
EVAP(-)/INFILT(+) RATE (CM/DAY):  8.2000E-02
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SURFACE BOUND LAYER (CM):         5.0000E-01
CLEAN COVER THICKNESS (CM):       0.0000E+00
 LAYER THICKNESS (CM)   CONTAM CONC (MG/KG)
          3.0000E+02              4.0000E+02

  EMSOFT RESULTS
  --------------
 Effective Diffusion Coefficient (cm**2/d)  1.868E+02
 Initial Mass for each Layer
Layer          Thickness (cm) Mass (mg/cm**2)
 1              3.000E+02      1.800E+02
AVERAGE FLUX FOR    1.095E+04 DAYS
  1.4668E-02
TOTAL FLUX FOR    1.095E+04 DAYS
  1.6062E+02
```

TIME (DAYS)	FLUX (MG/DAY/CM2)	AVG FLUX (MG/DAY/CM2)	CUM FLUX (MG/CM2)
2.50000E-01	9.22097E+00	1.83793E+01	4.59483E+00
1.09750E+02	2.78815E-01	7.50011E-01	8.67210E+01
2.19250E+02	1.24507E-01	1.84868E-01	1.06964E+02
3.28750E+02	7.35769E-02	9.53703E-02	1.17407E+02
4.38250E+02	4.98007E-02	6.04109E-02	1.24022E+02
5.47750E+02	3.65123E-02	4.25871E-02	1.28685E+02
6.57250E+02	2.82167E-02	3.20689E-02	1.32197E+02
7.66750E+02	2.26346E-02	2.52553E-02	1.34962E+02
8.76250E+02	1.86687E-02	2.05459E-02	1.37212E+02
9.85750E+02	1.57328E-02	1.71312E-02	1.39088E+02
1.09525E+03	1.34882E-02	1.45627E-02	1.40683E+02
1.20475E+03	1.17268E-02	1.25735E-02	1.42059E+02
1.31425E+03	1.03149E-02	1.09959E-02	1.43263E+02
1.42375E+03	9.16254E-03	9.71999E-03	1.44328E+02
1.53325E+03	8.20770E-03	8.67078E-03	1.45277E+02
1.64275E+03	7.40608E-03	7.79571E-03	1.46131E+02
1.75225E+03	6.72542E-03	7.05690E-03	1.46904E+02
1.86175E+03	6.14165E-03	6.42642E-03	1.47607E+02
1.97125E+03	5.63654E-03	5.88331E-03	1.48252E+02
2.08075E+03	5.19607E-03	5.41153E-03	1.48844E+02
2.19025E+03	4.80922E-03	4.99866E-03	1.49391E+02
2.29975E+03	4.46731E-03	4.63491E-03	1.49899E+02
2.40925E+03	4.16340E-03	4.31248E-03	1.50371E+02
2.51875E+03	3.89180E-03	4.02511E-03	1.50812E+02
2.62825E+03	3.64796E-03	3.76769E-03	1.51225E+02
2.73775E+03	3.42802E-03	3.53607E-03	1.51612E+02
2.84725E+03	3.22888E-03	3.32684E-03	1.51976E+02
2.95675E+03	3.04789E-03	3.13703E-03	1.52320E+02
3.06625E+03	2.88280E-03	2.96421E-03	1.52644E+02
3.17575E+03	2.73175E-03	2.80633E-03	1.52951E+02
3.28525E+03	2.59312E-03	2.66164E-03	1.53243E+02
3.39475E+03	2.46554E-03	2.52866E-03	1.53520E+02
3.50425E+03	2.34782E-03	2.40612E-03	1.53783E+02
3.61375E+03	2.23891E-03	2.29290E-03	1.54034E+02
3.72325E+03	2.13793E-03	2.18804E-03	1.54274E+02
3.83275E+03	2.04412E-03	2.09071E-03	1.54503E+02
3.94225E+03	1.95676E-03	2.00018E-03	1.54722E+02
4.05175E+03	1.87527E-03	1.91580E-03	1.54932E+02
4.16125E+03	1.79909E-03	1.83701E-03	1.55133E+02
4.27075E+03	1.72778E-03	1.76330E-03	1.55326E+02
4.38025E+03	1.66089E-03	1.69423E-03	1.55511E+02
4.48975E+03	1.59807E-03	1.62941E-03	1.55690E+02
4.59925E+03	1.53897E-03	1.56847E-03	1.55862E+02
4.70875E+03	1.48329E-03	1.51111E-03	1.56027E+02
4.81825E+03	1.43079E-03	1.45703E-03	1.56187E+02
4.92775E+03	1.38117E-03	1.40598E-03	1.56340E+02
5.03725E+03	1.33425E-03	1.35773E-03	1.56489E+02
5.14675E+03	1.28983E-03	1.31208E-03	1.56633E+02
5.25625E+03	1.24773E-03	1.26882E-03	1.56772E+02
5.36575E+03	1.20778E-03	1.22780E-03	1.56906E+02
5.47525E+03	1.16981E-03	1.18884E-03	1.57036E+02
5.58475E+03	1.13371E-03	1.15182E-03	1.57163E+02
5.69425E+03	1.09937E-03	1.11660E-03	1.57285E+02
5.80375E+03	1.06664E-03	1.08306E-03	1.57403E+02
5.91325E+03	1.03542E-03	1.05109E-03	1.57518E+02
6.02275E+03	1.00563E-03	1.02059E-03	1.57630E+02
6.13225E+03	9.77171E-04	9.91472E-04	1.57739E+02
6.24175E+03	9.49982E-04	9.63646E-04	1.57844E+02
6.35125E+03	9.23957E-04	9.37036E-04	1.57947E+02
6.46075E+03	8.99037E-04	9.11569E-04	1.58047E+02
6.57025E+03	8.75167E-04	8.87178E-04	1.58144E+02
6.67975E+03	8.52286E-04	8.63801E-04	1.58238E+02
6.78925E+03	8.30325E-04	8.41380E-04	1.58331E+02
6.89875E+03	8.09256E-04	8.19863E-04	1.58420E+02
7.00825E+03	7.88999E-04	7.99199E-04	1.58508E+02
7.11775E+03	7.69534E-04	7.79342E-04	1.58593E+02
7.22725E+03	7.50821E-04	7.60250E-04	1.58676E+02
7.33675E+03	7.32805E-04	7.41882E-04	1.58758E+02
7.44625E+03	7.15455E-04	7.24201E-04	1.58837E+02
7.55575E+03	6.98751E-04	7.07171E-04	1.58914E+02
7.66525E+03	6.82639E-04	6.90760E-04	1.58990E+02
7.77475E+03	6.67107E-04	6.74937E-04	1.59064E+02
7.88425E+03	6.52125E-04	6.59674E-04	1.59136E+02

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 7.99375E+03  6.37656E-04  6.44943E-04  1.59207E+02
 8.10325E+03  6.23680E-04  6.30719E-04  1.59276E+02
 8.21275E+03  6.10173E-04  6.16979E-04  1.59343E+02
 8.32225E+03  5.97118E-04  6.03699E-04  1.59410E+02
 8.43175E+03  5.84499E-04  5.90859E-04  1.59474E+02
 8.54125E+03  5.72281E-04  5.78439E-04  1.59538E+02
 8.65075E+03  5.60465E-04  5.66421E-04  1.59600E+02
 8.76025E+03  5.49019E-04  5.54785E-04  1.59660E+02
 8.86975E+03  5.37934E-04  5.43517E-04  1.59720E+02
 8.97925E+03  5.27188E-04  5.32599E-04  1.59778E+02
 9.08875E+03  5.16771E-04  5.22018E-04  1.59835E+02
 9.19825E+03  5.06678E-04  5.11758E-04  1.59891E+02
 9.30775E+03  4.96889E-04  5.01807E-04  1.59946E+02
 9.41725E+03  4.87362E-04  4.92152E-04  1.60000E+02
 9.52675E+03  4.78147E-04  4.82781E-04  1.60053E+02
 9.63625E+03  4.69170E-04  4.73683E-04  1.60105E+02
 9.74575E+03  4.60462E-04  4.64846E-04  1.60156E+02
 9.85525E+03  4.52010E-04  4.56261E-04  1.60206E+02
 9.96475E+03  4.43799E-04  4.47918E-04  1.60255E+02
 1.00742E+04  4.35786E-04  4.39807E-04  1.60303E+02
 1.01838E+04  4.28011E-04  4.31920E-04  1.60350E+02
 1.02932E+04  4.20443E-04  4.24248E-04  1.60397E+02
 1.04028E+04  4.13078E-04  4.16783E-04  1.60442E+02
 1.05122E+04  4.05917E-04  4.09517E-04  1.60487E+02
 1.06218E+04  3.98944E-04  4.02444E-04  1.60531E+02
 1.07312E+04  3.92151E-04  3.95557E-04  1.60575E+02
 1.08408E+04  3.85520E-04  3.88848E-04  1.60617E+02
  DEPTH (CM)  AVERAGE CONC (MG/KG)
 5.00000E+00  4.8501E-01
  TIME (DAYS)  AVERAGE CONC (MG/KG)
 2.50000E-01  8.18070E+01
 1.09750E+02  2.52934E+00
 2.19250E+02  1.12955E+00
 3.28750E+02  6.67513E-01
 4.38250E+02  4.51811E-01
 5.47750E+02  3.31254E-01
 6.57250E+02  2.55994E-01
 7.66750E+02  2.05350E-01
 8.76250E+02  1.69370E-01
 9.85750E+02  1.42735E-01
 1.09525E+03  1.22370E-01
 1.20475E+03  1.06390E-01
 1.31425E+03  9.35802E-02
 1.42375E+03  8.31258E-02
 1.53325E+03  7.44631E-02
 1.64275E+03  6.71906E-02
 1.75225E+03  6.10153E-02
 1.86175E+03  5.57191E-02
 1.97125E+03  5.11367E-02
 2.08075E+03  4.71405E-02
 2.19025E+03  4.36310E-02
 2.29975E+03  4.05292E-02
 2.40925E+03  3.77719E-02
 2.51875E+03  3.53079E-02
 2.62825E+03  3.30956E-02
 2.73775E+03  3.11004E-02
 2.84725E+03  2.92938E-02
 2.95675E+03  2.76518E-02
 3.06625E+03  2.61541E-02
 3.17575E+03  2.47838E-02
 3.28525E+03  2.35261E-02
 3.39475E+03  2.23687E-02
 3.50425E+03  2.13006E-02
 3.61375E+03  2.03127E-02
 3.72325E+03  1.93966E-02
 3.83275E+03  1.85455E-02
 3.94225E+03  1.77530E-02
 4.05175E+03  1.70136E-02
 4.16125E+03  1.63226E-02
 4.27075E+03  1.56756E-02
 4.38025E+03  1.50688E-02
 4.48975E+03  1.44989E-02
 4.59925E+03  1.39627E-02
 4.70875E+03  1.34577E-02
 4.81825E+03  1.29812E-02
 4.92775E+03  1.25312E-02
 5.03725E+03  1.21056E-02
 5.14675E+03  1.17026E-02
 5.25625E+03  1.13206E-02
 5.36575E+03  1.09581E-02
 5.47525E+03  1.06137E-02
 5.58475E+03  1.02862E-02
 5.69425E+03  9.97452E-03
 5.80375E+03  9.67757E-03
 5.91325E+03  9.39440E-03
 6.02275E+03  9.12415E-03
 6.13225E+03  8.86601E-03
 6.24175E+03  8.61924E-03
 6.35125E+03  8.38316E-03
 6.46075E+03  8.15714E-03
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 6.57025E+03  7.94059E-03
 6.67975E+03  7.73298E-03
 6.78925E+03  7.53379E-03
 6.89875E+03  7.34256E-03
 7.00825E+03  7.15887E-03
 7.11775E+03  6.98229E-03
 7.22725E+03  6.81247E-03
 7.33675E+03  6.64903E-03
 7.44625E+03  6.49167E-03
 7.55575E+03  6.34006E-03
 7.66525E+03  6.19392E-03
 7.77475E+03  6.05299E-03
 7.88425E+03  5.91700E-03
 7.99375E+03  5.78573E-03
 8.10325E+03  5.65894E-03
 8.21275E+03  5.53644E-03
 8.32225E+03  5.41802E-03
 8.43175E+03  5.30349E-03
 8.54125E+03  5.19269E-03
 8.65075E+03  5.08544E-03
 8.76025E+03  4.98160E-03
 8.86975E+03  4.88100E-03
 8.97925E+03  4.78353E-03
 9.08875E+03  4.68903E-03
 9.19825E+03  4.59740E-03
 9.30775E+03  4.50850E-03
 9.41725E+03  4.42224E-03
 9.52675E+03  4.33850E-03
 9.63625E+03  4.25718E-03
 9.74575E+03  4.17818E-03
 9.85525E+03  4.10143E-03
 9.96475E+03  4.02682E-03
 1.00742E+04  3.95428E-03
 1.01838E+04  3.88373E-03
 1.02932E+04  3.81509E-03
 1.04028E+04  3.74830E-03
 1.05122E+04  3.68328E-03
 1.06218E+04  3.61998E-03
 1.07312E+04  3.55833E-03
 1.08408E+04  3.49827E-03
  DEPTH (CM)   CONC (MG/KG)
 0.00000E+00  5.42963E-05
 1.00000E-01  1.89589E-04
 2.00000E-01  3.24894E-04
 3.00000E-01  4.60205E-04
 4.00000E-01  5.95522E-04
 5.00000E-01  7.30849E-04
 6.00000E-01  8.66184E-04
 7.00000E-01  1.00153E-03
 8.00000E-01  1.13688E-03
 9.00000E-01  1.27224E-03
 1.00000E+00  1.40760E-03
 1.10000E+00  1.54298E-03
 1.20000E+00  1.67835E-03
 1.30000E+00  1.81375E-03
 1.40000E+00  1.94914E-03
 1.50000E+00  2.08455E-03
 1.60000E+00  2.21996E-03
 1.70000E+00  2.35538E-03
 1.80000E+00  2.49082E-03
 1.90000E+00  2.62626E-03
 2.00000E+00  2.76170E-03
 2.10000E+00  2.89716E-03
 2.20000E+00  3.03262E-03
 2.30000E+00  3.16809E-03
 2.40000E+00  3.30356E-03
 2.50000E+00  3.43905E-03
 2.60000E+00  3.57454E-03
 2.70000E+00  3.71005E-03
 2.80000E+00  3.84556E-03
 2.90000E+00  3.98107E-03
 3.00000E+00  4.11660E-03
 3.10000E+00  4.25213E-03
 3.20000E+00  4.38767E-03
 3.30000E+00  4.52322E-03
 3.40000E+00  4.65878E-03
 3.50000E+00  4.79434E-03
 3.60000E+00  4.92992E-03
 3.70000E+00  5.06550E-03
 3.80000E+00  5.20109E-03
 3.90000E+00  5.33668E-03
 4.00000E+00  5.47229E-03
 4.10000E+00  5.60790E-03
 4.20000E+00  5.74352E-03
 4.30000E+00  5.87915E-03
 4.40000E+00  6.01479E-03
 4.50000E+00  6.15043E-03
 4.60000E+00  6.28609E-03
 4.70000E+00  6.42175E-03
 4.80000E+00  6.55742E-03
```

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4.90000E+00  6.69309E-03
5.00000E+00  6.82878E-03
```

Comparison to 124-Trichlorobenzene Benchmark Problem from EMSOFT Users Manual, Appendix B

Time (days)	Trichlorobenzene Surface Flux from Appendix A (mg/cm^2-d)	Trichlorobenzene Surface Flux from EMCONSOL2 (mg/cm^2-d)	Trichlorobenzene Average Concentration from Appendix A (mg/kg)	Trichlorobenzene Average Concentration from EMCONSOL2 (mg/kg)	Depth (m)	Trichlorobenzene Depth Concentration in Appendix A (mg/kg)	Trichlorobenzene Depth Concentration from EMCONSOL2 (mg/kg)
0.25	0.00E+00	0.00E+00	4.54E+01	4.59E+01	0	6.01E-02	6.01E-02
109.75	1.43E-05	1.43E-05	6.95E+01	6.97E+01	1.1	1.71E+00	1.71E+00
219.25	4.50E-04	4.50E-04	8.47E+01	8.49E+01	2.2	3.38E+00	3.38E+00
328.75	1.30E-03	1.30E-03	9.51E+01	9.53E+01	3.3	5.05E+00	5.05E+00
438.25	2.10E-03	2.10E-03	1.02E+02	1.03E+02	4.4	6.74E+00	6.74E+00
547.75	2.73E-03	2.73E-03	1.07E+02	1.08E+02	5.5	8.44E+00	8.44E+00
657.25	3.19E-03	3.19E-03	1.11E+02	1.11E+02	6.6	1.02E+01	1.02E+01
766.75	3.51E-03	3.51E-03	1.13E+02	1.13E+02	7.7	1.19E+01	1.19E+01
876.25	3.74E-03	3.74E-03	1.14E+02	1.14E+02	8.8	1.36E+01	1.36E+01
985.75	3.89E-03	3.89E-03	1.14E+02	1.15E+02	9.9	1.54E+01	1.54E+01
1095.25	3.99E-03	3.99E-03	1.14E+02	1.15E+02	11	1.71E+01	1.71E+01
1204.75	4.05E-03	4.05E-03	1.14E+02	1.14E+02	12.1	1.89E+01	1.89E+01
1314.25	4.08E-03	4.08E-03	1.13E+02	1.14E+02	13.2	2.07E+01	2.07E+01
1423.75	4.08E-03	4.08E-03	1.13E+02	1.13E+02	14.3	2.25E+01	2.25E+01
1533.25	4.08E-03	4.08E-03	1.12E+02	1.12E+02	15.4	2.43E+01	2.43E+01
1642.75	4.06E-03	4.06E-03	1.10E+02	1.11E+02	16.5	2.61E+01	2.61E+01
1752.25	4.03E-03	4.03E-03	1.09E+02	1.09E+02	17.6	2.79E+01	2.79E+01
1861.75	4.00E-03	4.00E-03	1.08E+02	1.08E+02	18.7	2.97E+01	2.97E+01
1971.25	3.96E-03	3.96E-03	1.07E+02	1.07E+02	19.8	3.16E+01	3.16E+01
2080.75	3.92E-03	3.92E-03	1.05E+02	1.05E+02	20.9	3.34E+01	3.34E+01
2190.25	3.88E-03	3.88E-03	1.04E+02	1.04E+02	22	3.53E+01	3.53E+01
2299.75	3.83E-03	3.83E-03	1.03E+02	1.03E+02	23.1	3.72E+01	3.72E+01
2409.25	3.78E-03	3.78E-03	1.01E+02	1.01E+02	24.2	3.90E+01	3.90E+01
2518.75	3.74E-03	3.74E-03	1.00E+02	1.00E+02	25.3	4.09E+01	4.09E+01
2628.25	3.69E-03	3.69E-03	9.86E+01	9.87E+01	26.4	4.28E+01	4.28E+01
2737.75	3.64E-03	3.64E-03	9.73E+01	9.74E+01	27.5	4.47E+01	4.47E+01
2847.25	3.59E-03	3.59E-03	9.61E+01	9.62E+01	28.6	4.67E+01	4.67E+01
2956.75	3.55E-03	3.55E-03	9.48E+01	9.49E+01	29.7	4.86E+01	4.86E+01
3066.25	3.50E-03	3.50E-03	9.36E+01	9.37E+01	30.8	5.05E+01	5.05E+01
3175.75	3.45E-03	3.45E-03	9.24E+01	9.24E+01	31.9	5.25E+01	5.25E+01
3285.25	3.41E-03	3.41E-03	9.12E+01	9.12E+01	33	5.44E+01	5.44E+01
3394.75	3.36E-03	3.36E-03	9.00E+01	9.01E+01	34.1	5.64E+01	5.64E+01
3504.25	3.32E-03	3.32E-03	8.88E+01	8.89E+01	35.2	5.84E+01	5.84E+01
3613.75	3.28E-03	3.28E-03	8.77E+01	8.78E+01	36.3	6.03E+01	6.03E+01
3723.25	3.23E-03	3.23E-03	8.66E+01	8.67E+01	37.4	6.23E+01	6.23E+01
3832.75	3.19E-03	3.19E-03	8.55E+01	8.56E+01	38.5	6.43E+01	6.43E+01
3942.25	3.15E-03	3.15E-03	8.45E+01	8.46E+01	39.6	6.63E+01	6.63E+01
4051.75	3.11E-03	3.11E-03	8.35E+01	8.35E+01	40.7	6.83E+01	6.83E+01
4161.25	3.07E-03	3.07E-03	8.25E+01	8.25E+01	41.8	7.04E+01	7.04E+01
4270.75	3.04E-03	3.04E-03	8.15E+01	8.15E+01	42.9	7.24E+01	7.24E+01
4380.25	3.00E-03	3.00E-03	8.05E+01	8.06E+01	44	7.44E+01	7.44E+01
4489.75	2.96E-03	2.96E-03	7.95E+01	7.96E+01	45.1	7.64E+01	7.64E+01
4599.25	2.93E-03	2.93E-03	7.86E+01	7.87E+01	46.2	7.85E+01	7.85E+01
4708.75	2.89E-03	2.89E-03	7.77E+01	7.78E+01	47.3	8.05E+01	8.05E+01
4818.25	2.86E-03	2.86E-03	7.68E+01	7.69E+01	48.4	8.26E+01	8.26E+01
4927.75	2.83E-03	2.83E-03	7.60E+01	7.60E+01	49.5	8.47E+01	8.47E+01

Time (days)	Trichlorobenzene Surface Flux from Appendix A (mg/cm^2-d)	Trichlorobenzene Surface Flux from EMCONSOL2 (mg/cm^2-d)	Trichlorobenzene Average Concentration from Appendix A (mg/kg)	Trichlorobenzene Average Concentration from EMCONSOL2 (mg/kg)	Depth (m)	Trichlorobenzene Depth Concentration in Appendix A (mg/kg)	Trichlorobenzene Depth Concentration from EMCONSOL2 (mg/kg)
5037.25	2.79E-03	2.79E-03	7.51E+01	7.52E+01	50.6	8.67E+01	8.67E+01
5146.75	2.76E-03	2.76E-03	7.43E+01	7.43E+01	51.7	8.88E+01	8.88E+01
5256.25	2.73E-03	2.73E-03	7.35E+01	7.35E+01	52.8	9.09E+01	9.09E+01
5365.75	2.70E-03	2.70E-03	7.27E+01	7.27E+01	53.9	9.30E+01	9.30E+01
5475.25	2.67E-03	2.67E-03	7.19E+01	7.19E+01			
5584.75	2.64E-03	2.64E-03	7.11E+01	7.12E+01			
5694.25	2.61E-03	2.61E-03	7.03E+01	7.04E+01			
5803.75	2.58E-03	2.58E-03	6.96E+01	6.97E+01			
5913.25	2.55E-03	2.55E-03	6.89E+01	6.89E+01			
6022.75	2.53E-03	2.53E-03	6.82E+01	6.82E+01			
6132.25	2.50E-03	2.50E-03	6.75E+01	6.75E+01			
6241.75	2.47E-03	2.47E-03	6.68E+01	6.68E+01			
6351.25	2.45E-03	2.45E-03	6.61E+01	6.62E+01			
6460.75	2.42E-03	2.42E-03	6.54E+01	6.55E+01			
6570.25	2.40E-03	2.40E-03	6.48E+01	6.48E+01			
6679.75	2.37E-03	2.37E-03	6.41E+01	6.42E+01			
6789.25	2.35E-03	2.35E-03	6.35E+01	6.36E+01			
6898.75	2.33E-03	2.33E-03	6.29E+01	6.30E+01			
7008.25	2.30E-03	2.30E-03	6.23E+01	6.24E+01			
7117.75	2.28E-03	2.28E-03	6.17E+01	6.18E+01			
7227.25	2.26E-03	2.26E-03	6.11E+01	6.12E+01			
7336.75	2.24E-03	2.24E-03	6.05E+01	6.06E+01			
7446.25	2.22E-03	2.22E-03	6.00E+01	6.00E+01			
7555.75	2.20E-03	2.20E-03	5.94E+01	5.95E+01			
7665.25	2.17E-03	2.17E-03	5.89E+01	5.89E+01			
7774.75	2.15E-03	2.15E-03	5.83E+01	5.84E+01			
7884.25	2.13E-03	2.13E-03	5.78E+01	5.79E+01			
7993.75	2.11E-03	2.11E-03	5.73E+01	5.73E+01			
8103.25	2.10E-03	2.10E-03	5.68E+01	5.68E+01			
8212.75	2.08E-03	2.08E-03	5.63E+01	5.63E+01			
8322.25	2.06E-03	2.06E-03	5.58E+01	5.58E+01			
8431.75	2.04E-03	2.04E-03	5.53E+01	5.53E+01			
8541.25	2.02E-03	2.02E-03	5.48E+01	5.48E+01			
8650.75	2.00E-03	2.00E-03	5.43E+01	5.44E+01			
8760.25	1.98E-03	1.98E-03	5.38E+01	5.39E+01			
8869.75	1.97E-03	1.97E-03	5.34E+01	5.34E+01			
8979.25	1.95E-03	1.95E-03	5.29E+01	5.30E+01			
9088.75	1.93E-03	1.93E-03	5.25E+01	5.25E+01			
9198.25	1.92E-03	1.92E-03	5.20E+01	5.21E+01			
9307.75	1.90E-03	1.90E-03	5.16E+01	5.16E+01			
9417.25	1.88E-03	1.88E-03	5.12E+01	5.12E+01			
9526.75	1.87E-03	1.87E-03	5.07E+01	5.08E+01			
9636.25	1.85E-03	1.85E-03	5.03E+01	5.04E+01			
9745.75	1.84E-03	1.84E-03	4.99E+01	4.99E+01			
9855.25	1.82E-03	1.82E-03	4.95E+01	4.95E+01			
9964.75	1.81E-03	1.81E-03	4.91E+01	4.91E+01			
10074.25	1.79E-03	1.79E-03	4.87E+01	4.87E+01			
10183.75	1.78E-03	1.78E-03	4.83E+01	4.83E+01			
10293.25	1.76E-03	1.76E-03	4.79E+01	4.80E+01			
10402.75	1.75E-03	1.75E-03	4.75E+01	4.76E+01			

Title: Air Pathway Assessment for the INL Remote-Handled Low-Level Waste Disposal Project

ECAR No.: 1370 ECAR Rev. No.: 1 Project File No.: NA Date: 09/28/2011

Time (days)	Trichlorobenzene Surface Flux from Appendix A (mg/cm^2-d)	Trichlorobenzene Surface Flux from EMCONSOL2 (mg/cm^2-d)	Trichlorobenzene Average Concentration from Appendix A (mg/kg)	Trichlorobenzene Average Concentration from EMCONSOL2 (mg/kg)	Depth (m)	Trichlorobenzene Depth Concentration in Appendix A (mg/kg)	Trichlorobenzene Depth Concentration from EMCONSOL2 (mg/kg)
10512.25	1.73E-03	1.73E-03	4.71E+01	4.72E+01			
10621.75	1.72E-03	1.72E-03	4.68E+01	4.68E+01			
10731.25	1.71E-03	1.71E-03	4.64E+01	4.65E+01			
10840.75	1.69E-03	1.69E-03	4.60E+01	4.61E+01			

124-Trichlorobenzene Benchmark Problem Input File for EMSOFT (Console Version)

```
124TRICHLOROBENZENE                                                                    READ(3,'(A25)')CHEM
  1.7800E+03     koc (mL/g)        KOC ORGANIC CARBON PARTITION COEFFICIENT            READ(3,*)KOC
  5.8200E-02     kh  (dimensionless henry's law)  HENRY'S LAW CONSTANT                 READ(3,*)KH
  2.5920E+03     Dair (cm2/day)    DVAIR   CHEMICAL DIFFUSION COEFF IN AIR             READ(3,*)DVAIR
  7.1107E-01     Dwat (cm2/day)    DLW     CHEMICAL DIFFUSION COEFF IN WATER           READ(3,*)DLW
  1.0000E+06     Thalf (days)      T12     CHEMICAL HALF LIFE                          READ(3,*)T12
      1          NLAY     NUMBER OF SOIL LAYERS                                        READ(3,*)NLAY
  5.5000E+01     ZP       DEPTH FOR PRINTING CONC RESULTS                              READ(3,*)ZP
  1.0950E+04  100   TP npnts      TIME FOR AVERAGING AND PRINTING FLUX AND CONC                 READ(3,*)TP npnts
  5.5050E+01     AVD1     DEPTH FOR AVERAGING CONC RESULTS                             READ(3,*)AVD1
  6.0000E-03     foc                                                                   READ(3,*)FOC
  4.3400E-01     phi                                                                   READ(3,*)PHI
  1.5000E-01     theta                                                                 READ(3,*)O
  1.5000E+00     rho                                                                   READ(3,*)PB
  8.2000E-02     E        VERTICAL POREWATER FLUX                                      READ(3,*)E
  5.0000E-01     surf bnd layer (cm)  DBL     BOUNDARY LAYER THICKNESS                 READ(3,*)DBL
  5.0000E+01     THICKNESS OF UNCONTAMINATED LAYER AT SURFACE                          READ(3,*)DC
  3.0000E+02     (DL(I),I=1,NLAY)  THICKNESS OF SOIL LAYER I                           READ(3,*)(DL(I),I=1,NLAY)
  5.0000E+02     (C0(I),I=1,NLAY)  CHEMICAL CONCENTRATIONS IN SOIL LAYER I             READ(3,*)(C0(I),I=1,NLAY)

  EMSOFT - Console Version 11-02-2010
  EMSOFT INPUT PARAMETERS
  -----------------------
CHEMICAL:                       124TRICHLOROBENZENE
KOC (ML/G):                       1.7800E+03
KH (DIMENSIONLESS):               5.8200E-02
AIR DIFF COEFF (CM2/DAY):         2.5920E+03
AQU DIFF COEFF (CM2/DAY):         7.1107E-01
HALF LIFE (DAYS):                 1.0000E+06
FRACTION ORG CARBON:              6.0000E-03
SOIL POROSITY:                    4.3400E-01
SOIL WATER CONTENT:               1.5000E-01
SOIL BULK DENSITY (G/CM3):        1.5000E+00
EVAP(-)/INFILT(+) RATE (CM/DAY):  8.2000E-02
SURFACE BOUND LAYER (CM):         5.0000E-01
CLEAN COVER THICKNESS (CM):       5.0000E+01
 LAYER THICKNESS (CM)   CONTAM CONC (MG/KG)
          3.0000E+02               5.0000E+02

  EMSOFT RESULTS
  --------------
 Effective Diffusion Coefficient (cm**2/d)  7.485E-01
 Initial Mass for each Layer
Layer          Thickness (cm) Mass (mg/cm**2)
 1               3.000E+02      2.250E+02
AVERAGE FLUX FOR    1.095E+04 DAYS
  2.6347E-03
TOTAL FLUX FOR    1.095E+04 DAYS
  2.8850E+01
   TIME        FLUX         AVG FLUX     CUM FLUX
  (DAYS)       (MG/DAY/CM2) (MG/DAY/CM2) (MG/CM2)
 2.50000E-01  0.00000E+00  0.00000E+00  0.00000E+00
 1.09750E+02  1.43085E-05  1.59465E-06  1.74614E-04
 2.19250E+02  4.50348E-04  1.76022E-04  1.94490E-02
 3.28750E+02  1.29758E-03  8.63843E-04  1.14040E-01
 4.38250E+02  2.10269E-03  1.71303E-03  3.01616E-01
 5.47750E+02  2.73056E-03  2.43208E-03  5.67929E-01
 6.57250E+02  3.18822E-03  2.97216E-03  8.93381E-01
 7.66750E+02  3.51193E-03  3.35969E-03  1.26127E+00
 8.76250E+02  3.73611E-03  3.63105E-03  1.65887E+00
 9.85750E+02  3.88749E-03  3.81691E-03  2.07682E+00
 1.09525E+03  3.98571E-03  3.94032E-03  2.50828E+00
 1.20475E+03  4.04498E-03  4.01807E-03  2.94826E+00
 1.31425E+03  4.07553E-03  4.06226E-03  3.39308E+00
 1.42375E+03  4.08484E-03  4.08167E-03  3.84002E+00
 1.53325E+03  4.07835E-03  4.08269E-03  4.28708E+00
 1.64275E+03  4.06010E-03  4.07004E-03  4.73275E+00
 1.75225E+03  4.03311E-03  4.04721E-03  5.17592E+00
 1.86175E+03  3.99964E-03  4.01682E-03  5.61576E+00
 1.97125E+03  3.96140E-03  3.98085E-03  6.05166E+00
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2.08075E+03  3.91971E-03  3.94080E-03  6.48318E+00
2.19025E+03  3.87557E-03  3.89781E-03  6.90999E+00
2.29975E+03  3.82976E-03  3.85278E-03  7.33187E+00
2.40925E+03  3.78286E-03  3.80638E-03  7.74867E+00
2.51875E+03  3.73535E-03  3.75914E-03  8.16029E+00
2.62825E+03  3.68758E-03  3.71148E-03  8.56670E+00
2.73775E+03  3.63984E-03  3.66370E-03  8.96788E+00
2.84725E+03  3.59233E-03  3.61606E-03  9.36383E+00
2.95675E+03  3.54522E-03  3.56874E-03  9.75461E+00
3.06625E+03  3.49865E-03  3.52189E-03  1.01403E+01
3.17575E+03  3.45270E-03  3.47563E-03  1.05208E+01
3.28525E+03  3.40746E-03  3.43003E-03  1.08964E+01
3.39475E+03  3.36296E-03  3.38515E-03  1.12671E+01
3.50425E+03  3.31925E-03  3.34105E-03  1.16329E+01
3.61375E+03  3.27636E-03  3.29775E-03  1.19941E+01
3.72325E+03  3.23430E-03  3.25525E-03  1.23505E+01
3.83275E+03  3.19307E-03  3.21363E-03  1.27024E+01
3.94225E+03  3.15268E-03  3.17281E-03  1.30498E+01
4.05175E+03  3.11312E-03  3.13283E-03  1.33929E+01
4.16125E+03  3.07439E-03  3.09369E-03  1.37316E+01
4.27075E+03  3.03647E-03  3.05536E-03  1.40662E+01
4.38025E+03  2.99935E-03  3.01784E-03  1.43966E+01
4.48975E+03  2.96301E-03  2.98112E-03  1.47231E+01
4.59925E+03  2.92745E-03  2.94517E-03  1.50456E+01
4.70875E+03  2.89264E-03  2.90998E-03  1.53642E+01
4.81825E+03  2.85856E-03  2.87554E-03  1.56791E+01
4.92775E+03  2.82521E-03  2.84183E-03  1.59903E+01
5.03725E+03  2.79255E-03  2.80882E-03  1.62978E+01
5.14675E+03  2.76056E-03  2.77650E-03  1.66019E+01
5.25625E+03  2.72925E-03  2.74485E-03  1.69024E+01
5.36575E+03  2.69857E-03  2.71385E-03  1.71996E+01
5.47525E+03  2.66852E-03  2.68349E-03  1.74934E+01
5.58475E+03  2.63907E-03  2.65374E-03  1.77840E+01
5.69425E+03  2.61022E-03  2.62460E-03  1.80714E+01
5.80375E+03  2.58194E-03  2.59603E-03  1.83557E+01
5.91325E+03  2.55421E-03  2.56803E-03  1.86369E+01
6.02275E+03  2.52703E-03  2.54057E-03  1.89151E+01
6.13225E+03  2.50037E-03  2.51365E-03  1.91903E+01
6.24175E+03  2.47422E-03  2.48725E-03  1.94627E+01
6.35125E+03  2.44856E-03  2.46135E-03  1.97322E+01
6.46075E+03  2.42338E-03  2.43593E-03  1.99989E+01
6.57025E+03  2.39867E-03  2.41099E-03  2.02629E+01
6.67975E+03  2.37441E-03  2.38650E-03  2.05242E+01
6.78925E+03  2.35060E-03  2.36247E-03  2.07829E+01
6.89875E+03  2.32721E-03  2.33887E-03  2.10390E+01
7.00825E+03  2.30423E-03  2.31568E-03  2.12926E+01
7.11775E+03  2.28166E-03  2.29291E-03  2.15437E+01
7.22725E+03  2.25948E-03  2.27054E-03  2.17923E+01
7.33675E+03  2.23768E-03  2.24855E-03  2.20385E+01
7.44625E+03  2.21626E-03  2.22694E-03  2.22824E+01
7.55575E+03  2.19519E-03  2.20570E-03  2.25239E+01
7.66525E+03  2.17448E-03  2.18481E-03  2.27631E+01
7.77475E+03  2.15411E-03  2.16427E-03  2.30001E+01
7.88425E+03  2.13407E-03  2.14406E-03  2.32349E+01
7.99375E+03  2.11435E-03  2.12419E-03  2.34675E+01
8.10325E+03  2.09495E-03  2.10463E-03  2.36979E+01
8.21275E+03  2.07586E-03  2.08538E-03  2.39263E+01
8.32225E+03  2.05707E-03  2.06644E-03  2.41526E+01
8.43175E+03  2.03857E-03  2.04780E-03  2.43768E+01
8.54125E+03  2.02035E-03  2.02944E-03  2.45990E+01
8.65075E+03  2.00241E-03  2.01136E-03  2.48193E+01
8.76025E+03  1.98474E-03  1.99356E-03  2.50376E+01
8.86975E+03  1.96734E-03  1.97602E-03  2.52539E+01
8.97925E+03  1.95019E-03  1.95875E-03  2.54684E+01
9.08875E+03  1.93329E-03  1.94173E-03  2.56810E+01
9.19825E+03  1.91664E-03  1.92496E-03  2.58918E+01
9.30775E+03  1.90023E-03  1.90843E-03  2.61008E+01
9.41725E+03  1.88406E-03  1.89214E-03  2.63080E+01
9.52675E+03  1.86811E-03  1.87608E-03  2.65134E+01
9.63625E+03  1.85239E-03  1.86024E-03  2.67171E+01
9.74575E+03  1.83688E-03  1.84463E-03  2.69191E+01
9.85525E+03  1.82159E-03  1.82923E-03  2.71194E+01
9.96475E+03  1.80651E-03  1.81404E-03  2.73180E+01
1.00742E+04  1.79163E-03  1.79906E-03  2.75150E+01
1.01838E+04  1.77696E-03  1.78428E-03  2.77104E+01
1.02932E+04  1.76247E-03  1.76971E-03  2.79042E+01
1.04028E+04  1.74818E-03  1.75532E-03  2.80964E+01
1.05122E+04  1.73408E-03  1.74112E-03  2.82871E+01
1.06218E+04  1.72017E-03  1.72711E-03  2.84762E+01
1.07312E+04  1.70643E-03  1.71329E-03  2.86638E+01
1.08408E+04  1.69287E-03  1.69964E-03  2.88499E+01
 DEPTH (CM)  AVERAGE CONC (MG/KG)
5.50500E+01  7.4981E+01
 TIME (DAYS)  AVERAGE CONC (MG/KG)
2.50000E-01  4.58522E+01
1.09750E+02  6.97000E+01
2.19250E+02  8.48531E+01
3.28750E+02  9.53012E+01
4.38250E+02  1.02557E+02
5.47750E+02  1.07517E+02
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6.57250E+02	1.10809E+02
7.66750E+02	1.12879E+02
8.76250E+02	1.14047E+02
9.85750E+02	1.14547E+02
1.09525E+03	1.14547E+02
1.20475E+03	1.14173E+02
1.31425E+03	1.13521E+02
1.42375E+03	1.12661E+02
1.53325E+03	1.11646E+02
1.64275E+03	1.10518E+02
1.75225E+03	1.09309E+02
1.86175E+03	1.08043E+02
1.97125E+03	1.06738E+02
2.08075E+03	1.05411E+02
2.19025E+03	1.04071E+02
2.29975E+03	1.02728E+02
2.40925E+03	1.01389E+02
2.51875E+03	1.00059E+02
2.62825E+03	9.87417E+01
2.73775E+03	9.74411E+01
2.84725E+03	9.61591E+01
2.95675E+03	9.48975E+01
3.06625E+03	9.36576E+01
3.17575E+03	9.24403E+01
3.28525E+03	9.12461E+01
3.39475E+03	9.00753E+01
3.50425E+03	8.89281E+01
3.61375E+03	8.78043E+01
3.72325E+03	8.67039E+01
3.83275E+03	8.56266E+01
3.94225E+03	8.45720E+01
4.05175E+03	8.35398E+01
4.16125E+03	8.25295E+01
4.27075E+03	8.15407E+01
4.38025E+03	8.05728E+01
4.48975E+03	7.96253E+01
4.59925E+03	7.86978E+01
4.70875E+03	7.77897E+01
4.81825E+03	7.69005E+01
4.92775E+03	7.60297E+01
5.03725E+03	7.51767E+01
5.14675E+03	7.43411E+01
5.25625E+03	7.35224E+01
5.36575E+03	7.27200E+01
5.47525E+03	7.19336E+01
5.58475E+03	7.11625E+01
5.69425E+03	7.04065E+01
5.80375E+03	6.96650E+01
5.91325E+03	6.89377E+01
6.02275E+03	6.82241E+01
6.13225E+03	6.75238E+01
6.24175E+03	6.68365E+01
6.35125E+03	6.61617E+01
6.46075E+03	6.54991E+01
6.57025E+03	6.48484E+01
6.67975E+03	6.42093E+01
6.78925E+03	6.35813E+01
6.89875E+03	6.29642E+01
7.00825E+03	6.23577E+01
7.11775E+03	6.17616E+01
7.22725E+03	6.11754E+01
7.33675E+03	6.05990E+01
7.44625E+03	6.00321E+01
7.55575E+03	5.94744E+01
7.66525E+03	5.89257E+01
7.77475E+03	5.83858E+01
7.88425E+03	5.78544E+01
7.99375E+03	5.73314E+01
8.10325E+03	5.68164E+01
8.21275E+03	5.63094E+01
8.32225E+03	5.58100E+01
8.43175E+03	5.53182E+01
8.54125E+03	5.48337E+01
8.65075E+03	5.43563E+01
8.76025E+03	5.38860E+01
8.86975E+03	5.34225E+01
8.97925E+03	5.29656E+01
9.08875E+03	5.25152E+01
9.19825E+03	5.20712E+01
9.30775E+03	5.16335E+01
9.41725E+03	5.12018E+01
9.52675E+03	5.07760E+01
9.63625E+03	5.03560E+01
9.74575E+03	4.99418E+01
9.85525E+03	4.95331E+01
9.96475E+03	4.91298E+01
1.00742E+04	4.87319E+01
1.01838E+04	4.83392E+01
1.02932E+04	4.79516E+01
1.04028E+04	4.75690E+01

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 1.05122E+04  4.71913E+01
 1.06218E+04  4.68184E+01
 1.07312E+04  4.64503E+01
 1.08408E+04  4.60867E+01
  DEPTH (CM)  CONC (MG/KG)
 0.00000E+00  6.00698E-02
 1.10000E+00  1.71199E+00
 2.20000E+00  3.37606E+00
 3.30000E+00  5.05217E+00
 4.40000E+00  6.74022E+00
 5.50000E+00  8.44009E+00
 6.60000E+00  1.01517E+01
 7.70000E+00  1.18749E+01
 8.80000E+00  1.36096E+01
 9.90000E+00  1.53557E+01
 1.10000E+01  1.71130E+01
 1.21000E+01  1.88815E+01
 1.32000E+01  2.06610E+01
 1.43000E+01  2.24515E+01
 1.54000E+01  2.42527E+01
 1.65000E+01  2.60645E+01
 1.76000E+01  2.78868E+01
 1.87000E+01  2.97196E+01
 1.98000E+01  3.15626E+01
 2.09000E+01  3.34157E+01
 2.20000E+01  3.52788E+01
 2.31000E+01  3.71517E+01
 2.42000E+01  3.90343E+01
 2.53000E+01  4.09265E+01
 2.64000E+01  4.28281E+01
 2.75000E+01  4.47390E+01
 2.86000E+01  4.66589E+01
 2.97000E+01  4.85879E+01
 3.08000E+01  5.05256E+01
 3.19000E+01  5.24720E+01
 3.30000E+01  5.44270E+01
 3.41000E+01  5.63902E+01
 3.52000E+01  5.83617E+01
 3.63000E+01  6.03412E+01
 3.74000E+01  6.23286E+01
 3.85000E+01  6.43236E+01
 3.96000E+01  6.63262E+01
 4.07000E+01  6.83362E+01
 4.18000E+01  7.03534E+01
 4.29000E+01  7.23776E+01
 4.40000E+01  7.44087E+01
 4.51000E+01  7.64465E+01
 4.62000E+01  7.84907E+01
 4.73000E+01  8.05414E+01
 4.84000E+01  8.25982E+01
 4.95000E+01  8.46610E+01
 5.06000E+01  8.67295E+01
 5.17000E+01  8.88038E+01
 5.28000E+01  9.08834E+01
 5.39000E+01  9.29684E+01
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Appendix C, EMSOFT Input Files (Console Version) for the RH-LLW Air Pathway Analysis

C-14.par

```
C-14 modeled as C02 for RHLLW                                                          READ(3,'(A25)')CHEM
  0.5            koc (mL/g)        KOC ORGANIC CARBON PARTITION COEFFICIENT            READ(3,*)KOC

$ Inverse Henry's law (Hinv) from Denham 2010
$ Hinv = 2.8  mol/kg-atm  rho water = 1 kg/L, R = 0.082 atm-L/mol-K, T = 289 K
$ H dimensionless = 1/(Hinv x rho x RT)
  0.0151E-00     kh (dimensionless henry's law)  HENRY'S LAW CONSTANT                  READ(3,*)KH

$ Dair and Dwat from EPA diffusion coeff calculator http://www.epa.gov/athens/learn2model/part-two/onsite/estdiffusion-ext.html
  1.3200E+04     Dair (cm2/day)    DVAIR   CHEMICAL DIFFUSION COEFF IN AIR             READ(3,*)DVAIR
  1.3400E-00     Dwat (cm2/day)    DLW     CHEMICAL DIFFUSION COEFF IN WATER           READ(3,*)DLW

$ C-14 half life 5700 years (2.08E6 days)
  2.0800E+06     Thalf (days)      T12     CHEMICAL HALF LIFE                          READ(3,*)T12
  2              NLAY     NUMBER OF SOIL LAYERS                                        READ(3,*)NLAY
  6.0000E+02     ZP  (cm) DEPTH FOR PRINTING CONC RESULTS                              READ(3,*)ZP

 200 years * 365 days 73000
  73000 2000     TP (days) TIME FOR AVERAGING AND PRINTING FLUX AND CONC               READ(3,*)TP nponts
  3.0000E+02     AVD1 (cm) DEPTH FOR AVERAGING CONC RESULTS                            READ(3,*)AVD1

$ foc and koc are set so that kd=koc
$ phi and theta are based on waste properties
  1.0000E-00     foc                                                                   READ(3,*)FOC
  3.2000E-01     phi   (total porosity)                                                READ(3,*)PHI
  0.0726E-01     theta (moisture content)                                              READ(3,*)O
  1.8200E+00     rho   (g/cc)                                                          READ(3,*)PB

$ Vertical porewater flux is based on 1 cm/yr
  2.7400E-03     E     (cm/d)   VERTICAL POREWATER FLUX  (cm/d)                        READ(3,*)E
  4.2200E-01     surf bnd layer (cm)  DBL  BOUNDARY LAYER THICKNESS                    READ(3,*)DBL

$ cover thickness based on 1 m of soil during operations
  1.0000E+02     THICKNESS OF UNCONTAMINATED LAYER AT SURFACE                          READ(3,*)DC

$ 6.0 m waste layer and 18 m below
  6.0000E+02 1.80E4  (DL(I),I=1,NLAY) THICKNESS OF SOIL LAYER I    (cm)                READ(3,*)(DL(I),I=1,NLAY)
  1.0000E+00 0.0     (C0(I),I=1,NLAY) CHEMICAL CONCENTRATIONS IN SOIL LYR I (mg/kg)    READ(3,*)(C0(I),I=1,NLAY)

C     CHEM    CHAR*25 CHEMICAL NAME
C     KOC     REAL*8  ORGANIC CARBON PARTITION COEFFICIENT
C     KH      REAL*8  HENRYS LAW CONSTANT
C     DVAIR   REAL*8  CHEMICAL DIFFUSION COEFF IN AIR
C     DLW     REAL*8  CHEMICAL DIFFUSION COEFF IN WATER
C     T12     REAL*8  CHEMICAL HALF LIFE
C     NLAY    INT     NUMBER OF SOIL LAYERS
C     ZP      REAL*8  DEPTH FOR PRINTING CONC RESULTS
C     FOC     REAL*8  SOIL FRACTION ORGANIC CARBON
C     O       REAL*8  SOIL WATER CONTENT
C     PB      REAL*8  SOIL BULK DENSITY
C     E       REAL*8  VERTICAL POREWATER FLUX
C     DBL     REAL*8  BOUNDARY LAYER THICKNESS
C     DL(I)   REAL*8  THICKNESS OF SOIL LAYER I
C     C0(I)   REAL*8  CHEMICAL CONCENTRATIONS IN SOIL LAYER I
C     TP      REAL*8  TIME FOR AVERAGING AND PRINTING FLUX AND CONC
C     AVD1    REAL*8  DEPTH FOR AVERAGING CONC RESULTS
C     DC      REAL*8  THICKNESS OF UNCONTAMINATED LAYER AT SURFACE
C     L1(I)   REAL*8  DEPTH OF TOP OF SOIL LAYER I
C     L(I)    REAL*8  DEPTH OF BOTTOM OF SOIL LAYER I
C     DT      REAL*8  TIME INTERVAL
C     IC,ICT  INT     IC OR ICT=1 FOR T<T0, IC OR ICT=2 FOR T>T0
C     II      INT     COUNTER FOR TIME VECTOR
```

H-3.par

```
Tritium modeled as HT or T2
  0.0000E-00     koc (mL/g)        KOC ORGANIC CARBON PARTITION COEFFICIENT            READ(3,*)KOC

$ Inverse Henry's law (Hinv) from Sander (1999)
$ Hinv = 7.8E-4 mol/L-atm  R = 0.082 atm-L/mol, T = 288 K
$ H dimensionless = 1/(Hinv x RT)
  54.20          kh  (dimensionless henry's law)  HENRY'S LAW CONSTANT                 READ(3,*)KH

$ Dair and Dwat from EPA diffusion coeff calculator http://www.epa.gov/athens/learn2model/part-two/onsite/estdiffusion-ext.html
  6.8600E+04     Dair (cm2/day)    DVAIR   CHEMICAL DIFFUSION COEFF IN AIR             READ(3,*)DVAIR
  3.0400E+00     Dwat (cm2/day)    DLW     CHEMICAL DIFFUSION COEFF IN WATER           READ(3,*)DLW

$ H-3   half life 12.3 yr years (4489.5 days)
  4.4895E+03     Thalf (days)      T12     CHEMICAL HALF LIFE                          READ(3,*)T12
  2              NLAY     NUMBER OF SOIL LAYERS                                        READ(3,*)NLAY
  6.0000E+02     ZP  (cm) DEPTH FOR PRINTING CONC RESULTS                              READ(3,*)ZP

$ 200 years * 365 days 73000
```

```
  73000 2000      TP (days) TIME FOR AVERAGING AND PRINTING FLUX AND CONC          READ(3,*)TP nponts
  3.0000E+02      AVD1 (cm) DEPTH FOR AVERAGING CONC RESULTS                       READ(3,*)AVD1

$ foc and koc are set so koc=kd
$ phi and theta are based on waste properties
  1.0000E-00     foc                                                               READ(3,*)FOC
  3.2000E-01     phi   (total porosity)                                            READ(3,*)PHI
  0.0726E-01     theta (moisture content)                                          READ(3,*)O
  1.8200E+00     rho   (g/cc)                                                      READ(3,*)PB

$ Vertical porewater flux is based on 1 cm/yr
  2.7400E-03     E     (cm/d)   VERTICAL POREWATER FLUX                            READ(3,*)E
  2.4400E-01     surf bnd layer (cm)  DBL  BOUNDARY LAYER THICKNESS                READ(3,*)DBL

$ Thickness of cover above waste based on cover design
  1.0000E+02    THICKNESS OF UNCONTAMINATED LAYER AT SURFACE   (cm)                READ(3,*)DC

$ 6.0 m waste layer and 18 m below
  6.0000E+02 1.80E4  (DL(I),I=1,NLAY) THICKNESS OF SOIL LAYER I    (cm)            READ(3,*)(DL(I),I=1,NLAY)
  1.0000E+00 0.0    (C0(I),I=1,NLAY) CHEMICAL CONCENTRATIONS IN SOIL LYR I (mg/kg)  READ(3,*)(C0(I),I=1,NLAY)

C     CHEM    CHAR*25 CHEMICAL NAME
C     KOC     REAL*8  ORGANIC CARBON PARTITION COEFFICIENT
C     KH      REAL*8  HENRYS LAW CONSTANT
C     DVAIR   REAL*8  CHEMICAL DIFFUSION COEFF IN AIR
C     DLW     REAL*8  CHEMICAL DIFFUSION COEFF IN WATER
C     T12     REAL*8  CHEMICAL HALF LIFE
C     NLAY    INT     NUMBER OF SOIL LAYERS
C     ZP      REAL*8  DEPTH FOR PRINTING CONC RESULTS
C     FOC     REAL*8  SOIL FRACTION ORGANIC CARBON
C     O       REAL*8  SOIL WATER CONTENT
C     PB      REAL*8  SOIL BULK DENSITY
C     E       REAL*8  VERTICAL POREWATER FLUX
C     DBL     REAL*8  BOUNDARY LAYER THICKNESS
C     DL(I)   REAL*8  THICKNESS OF SOIL LAYER I
C     C0(I)   REAL*8  CHEMICAL CONCENTRATIONS IN SOIL LAYER I
C     TP      REAL*8  TIME FOR AVERAGING AND PRINTING FLUX AND CONC
C     AVD1    REAL*8  DEPTH FOR AVERAGING CONC RESULTS
C     DC      REAL*8  THICKNESS OF UNCONTAMINATED LAYER AT SURFACE
C     L1(I)   REAL*8  DEPTH OF TOP OF SOIL LAYER I
C     L(I)    REAL*8  DEPTH OF BOTTOM OF SOIL LAYER I
C     DT      REAL*8  TIME INTERVAL
C     IC,ICT  INT     IC OR ICT=1 FOR T<T0, IC OR ICT=2 FOR T>T0
C     II      INT     COUNTER FOR TIME VECTORS
```

I-129.par

```
I-129 modeled as I2                                                                READ(3,'(A25)')CHEM
  3.0000E-00     koc (mL/g)        KOC ORGANIC CARBON PARTITION COEFFICIENT        READ(3,*)KOC

$ Inverse Henry's law (Hinv) from Sander (1999)
$ Hinv = 1.1 mol/L-atm  R = 0.082 atm-L/mol, T = 288 K
$ H dimensionless = 1/(Hinv x RT)

  0.0384     kh  (dimensionless henry's law)  HENRY'S LAW CONSTANT                 READ(3,*)KH

$ Dair and Dwat from EPA diffusion coeff calculator http://www.epa.gov/athens/learn2model/part-two/onsite/estdiffusion-ext.html
  7.5300E+03     Dair (cm2/day)    DVAIR   CHEMICAL DIFFUSION COEFF IN AIR         READ(3,*)DVAIR
  7.8300E-01     Dwat (cm2/day)    DLW     CHEMICAL DIFFUSION COEFF IN WATER       READ(3,*)DLW

$ I-129 half life 1.57E7 yr years (5.73E9 days)
  5.7300E+09     Thalf (days)      T12     CHEMICAL HALF LIFE                      READ(3,*)T12
  2              NLAY     NUMBER OF SOIL LAYERS                                    READ(3,*)NLAY
  6.0000E+02     ZP  (cm) DEPTH FOR PRINTING CONC RESULTS                          READ(3,*)ZP

$ 200 years * 365 days 73000
  73000 2000     TP (days) TIME FOR AVERAGING AND PRINTING FLUX AND CONC           READ(3,*)TP nponts
  3.0000E+02     AVD1 (cm) DEPTH FOR AVERAGING CONC RESULTS                        READ(3,*)AVD1

$ foc and koc are set so that a koc=kd
$ phi and theta are based on waste properties
  1.0000E-00     foc                                                               READ(3,*)FOC
  3.2000E-01     phi   (total porosity)                                            READ(3,*)PHI
  0.0726E-01     theta (moisture content)                                          READ(3,*)O
  1.8200E+00     rho   (g/cc)                                                      READ(3,*)PB

$ Vertical porewater flux is based on 1 cm/yr
  2.7400E-03     E     (cm/d)   VERTICAL POREWATER FLUX                            READ(3,*)E
  5.0900E-01     surf bnd layer (cm)  DBL  BOUNDARY LAYER THICKNESS                READ(3,*)DBL

$ Cover thickness based on ICDF cover design
  1.0000E+02    THICKNESS OF UNCONTAMINATED LAYER AT SURFACE   (cm)                READ(3,*)DC

$ 6.0 m waste layer and 18 m below
  6.0000E+02 1.80E4  (DL(I),I=1,NLAY) THICKNESS OF SOIL LAYER I    (cm)            READ(3,*)(DL(I),I=1,NLAY)
  1.0000E+00 0.0    (C0(I),I=1,NLAY) CHEMICAL CONCENTRATIONS IN SOIL LYR I (mg/kg)  READ(3,*)(C0(I),I=1,NLAY)

C     CHEM    CHAR*25 CHEMICAL NAME
C     KOC     REAL*8  ORGANIC CARBON PARTITION COEFFICIENT
```

```
C     KH      REAL*8  HENRYS LAW CONSTANT
C     DVAIR   REAL*8  CHEMICAL DIFFUSION COEFF IN AIR
C     DLW     REAL*8  CHEMICAL DIFFUSION COEFF IN WATER
C     T12     REAL*8  CHEMICAL HALF LIFE
C     NLAY    INT     NUMBER OF SOIL LAYERS
C     ZP      REAL*8  DEPTH FOR PRINTING CONC RESULTS
C     FOC     REAL*8  SOIL FRACTION ORGANIC CARBON
C     O       REAL*8  SOIL WATER CONTENT
C     PB      REAL*8  SOIL BULK DENSITY
C     E       REAL*8  VERTICAL POREWATER FLUX
C     DBL     REAL*8  BOUNDARY LAYER THICKNESS
C     DL(I)   REAL*8  THICKNESS OF SOIL LAYER I
C     C0(I)   REAL*8  CHEMICAL CONCENTRATIONS IN SOIL LAYER I
C     TP      REAL*8  TIME FOR AVERAGING AND PRINTING FLUX AND CONC
C     AVD1    REAL*8  DEPTH FOR AVERAGING CONC RESULTS
C     DC      REAL*8  THICKNESS OF UNCONTAMINATED LAYER AT SURFACE
C     L1(I)   REAL*8  DEPTH OF TOP OF SOIL LAYER I
C     L(I)    REAL*8  DEPTH OF BOTTOM OF SOIL LAYER I
C     DT      REAL*8  TIME INTERVAL
C     IC,ICT  INT     IC OR ICT=1 FOR T<T0, IC OR ICT=2 FOR T>T0
C     II      INT     COUNTER FOR TIME VECTORS
```

Appendix D, RESRAD Input File

```
&DB
 HAFTIM = '180 days',
 EXTERNAL_DCF= 'FGR 12',
 DFFILE = 'FGR 13 Morbidity',
 RISKLIB= 'FGR 13 Morbidity',
 DOSELIB= 'FGR 11',
 NANUC =  9 ,
 NIY =  7 ,
 NPD =  24 ,
 NPTS =  32 ,
 NS =  1 ,
 NPDS =  25 ,
 U_activity = 'pCi' ,
 U_dose_unit = 'mrem' ,
 nDAll =  3 ,
 nUniqueNuc =  18 ,
 &END
 &INDATA
 TITLE = 'BEA RH-LLW RADON PA 2011',
 NPTS = 32 ,
 TDISK = '', VERS = '6.5',
 XSPACE = 'LOG',
 FINDPEAK = 1 ,
 LYMAX = 17 ,
 KYMAX = 257 ,
 COVER0 = 1,
 DENSCV = 1.82,
 VCV = 0,
 DENSCZ = 1.82,
 VCZ = 0,
 TPCZ = .32,
 FCCZ = .2,
 HCCZ = 10,
 BCZ = 5.3,
 HUMID = 8,
 EVAPTR = .5,
 PRECIP = .2212,
 RI = 0,
 IDITCH = 0,
 RUNOFF = .2,
 WAREA = 1000000,
 EPS = .001,
 NS = 1,
 TI = 0,
 DENSAQ = 1.5,
 TPSZ = .4,
 EPSZ = .2,
 FCSZ = .2,
 HCSZ = 100,
 HGWT = .02,
 BSZ = 5.3,
 VWT = .001,
 DWIBWT = 10,
 MODEL = 0,
 UW = 250,
 AREA = 2400,
 THICK0 = 6,
 SUBMFRACT = 0,
 LCZPAQ = 100,
 BRDL = 25,
 T(1) = 0,
 T(2) = 1,
 T(3) = 100,
 T(4) = 300,
 T(5) = 500,
 T(6) = 1000,
 T(7) = 10000,
 T(8) = 0,
 T(9) = 0,
 T(10) = 0,
 INHALR = 8400,
 MLINH = .0001,
 ED = 30,
 SHF1 = .7,
 SHF3 = .4,
 FIND = .5,
 FOTD = .25,
 FS = 1,
 RAD_SHAPE(1) = 50,
 RAD_SHAPE(2) = 70.71068,
 RAD_SHAPE(3) = 0,
 RAD_SHAPE(4) = 0,
 RAD_SHAPE(5) = 0,
 RAD_SHAPE(6) = 0,
 RAD_SHAPE(7) = 0,
 RAD_SHAPE(8) = 0,
 RAD_SHAPE(9) = 0,
```

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RAD_SHAPE(10) = 0,
RAD_SHAPE(11) = 0,
RAD_SHAPE(12) = 0,
FRACA(1) = 1,
FRACA(2) = .2732395,
FRACA(3) = 0,
FRACA(4) = 0,
FRACA(5) = 0,
FRACA(6) = 0,
FRACA(7) = 0,
FRACA(8) = 0,
FRACA(9) = 0,
FRACA(10) = 0,
FRACA(11) = 0,
FRACA(12) = 0,
DIET(1) = 160,
DIET(2) = 14,
DIET(3) = 92,
DIET(4) = 63,
DIET(5) = 5.4,
DIET(6) = .9,
SOIL = 36.5,
DWI = 510,
FDW = 1,
FHHW = 1,
FLW = 1,
FIRW = 1,
FR9 = .5,
FPLANT =-1,
FMEAT =-1,
FMILK =-1,
LFI5 = 68,
LFI6 = 55,
LWI5 = 50,
LWI6 = 160,
LSI = .5,
MLFD = .0001,
DM = .15,
DROOT = .9,
FGWDW = 1,
FGWHH = 1,
FGWLW = 1,
FGWIR = 1,
STOR_T(1) = 14,
STOR_T(2) = 1,
STOR_T(3) = 1,
STOR_T(4) = 20,
STOR_T(5) = 7,
STOR_T(6) = 7,
STOR_T(7) = 1,
STOR_T(8) = 1,
STOR_T(9) = 45,
FLOOR1 = .15,
DENSFL = 2.4,
TPCV = .32,
TPFL = .1,
PH2OCV = .0726,
PH2OFL = .03,
DIFCV = .000002,
DIFFL = .0000003,
DIFCZ = .000002,
HMIX = 2,
WIND = 3.35,
REXG = .5,
HRM = 2.5,
FAI = 0,
DMFL =-1,
EMANA(1) = .25,
EMANA(2) = .15,
C12WTR = .00002,
C12CZ = .03,
CSOIL = .02,
CAIR = .98,
DMC = .3,
EVSN = .0000007,
REVSN = 1E-10,
AVFG4 = .8,
AVFG5 = .2,
H(1) = 4,
H(2) = 4,
H(3) = 4,
H(4) = 4,
H(5) = 4,
DENSUZ(1) = 1.82,
DENSUZ(2) = 1.5,
DENSUZ(3) = 1.5,
DENSUZ(4) = 1.5,
DENSUZ(5) = 1.5,
TPUZ(1) = .32,
TPUZ(2) = .4,
```

```
TPUZ(3) = .4,
TPUZ(4) = .4,
TPUZ(5) = .4,
EPUZ(1) = .2,
EPUZ(2) = .2,
EPUZ(3) = .2,
EPUZ(4) = .2,
EPUZ(5) = .2,
FCUZ(1) = .2,
FCUZ(2) = .2,
FCUZ(3) = .2,
FCUZ(4) = .2,
FCUZ(5) = .2,
BUZ(1) = 5.3,
BUZ(2) = 5.3,
BUZ(3) = 5.3,
BUZ(4) = 5.3,
BUZ(5) = 5.3,
HCUZ(1) = 10,
HCUZ(2) = 10,
HCUZ(3) = 10,
HCUZ(4) = 10,
HCUZ(5) = 10,
INDPOPFLAG = 0,
OFFDISTANCE(1) = 250,
NUMDISTANCES = 0,
AMBIENTTEMP = 10,
LIDHEIGHT = 1000,
SOURCEHEIGHT = 10,
AGVEG(1) = 0,
AGVEG(2) = .5,
AGVEG(3) = .5,
AGMILK(1) = 0,
AGMILK(2) = .5,
AGMILK(3) = .5,
AGMEAT(1) = 0,
AGMEAT(2) = .5,
AGMEAT(3) = .5,
BEEFDENSITY = .164,
MILKDENSITY = .0207,
VEGLANDFRACTION = .0185,
YV(1) = .7,
YV(2) = 1.5,
YV(3) = 1.1,
TE(1) = .17,
TE(2) = .25,
TE(3) = .08,
TIV(1) = .1,
TIV(2) = 1,
TIV(3) = 1,
WLAM = 20,
RWET(1) = .25,
RWET(2) = .25,
RWET(3) = .25,
RDRY(1) = .25,
RDRY(2) = .25,
RDRY(3) = .25,
NUCNAM = 'Pb-210+D', 'Pu-242', 'Pu-242', 'Pu-242', 'Ra-226+D',
'Th-230', 'U-234', 'U-238', 'U-238+D', 'LAST',
S = 0, 3*.0153, .0000000031, .0000026, .0458, 2*618,
W = 9*0,
DCACTC = 100, 3*2000, 70, 60000, 3*50,
DCACTU1 = 100, 3*2000, 70, 60000, 3*50,
DCACTS = 100, 3*2000, 70, 60000, 3*50,
RLEACH = 9*0,
SOLUBK0 = 9*0,
NSENA = 0,
NUM_SAMPS = 300, NUMVAR = 3,
UNCPPD = 1 ,
UNCPND = 1 ,
SELPATH = 256,
&END
&DCF
T_DCF2= .023196, 0.411, 0.411, 0.411, 8.594398E-03, 0.326, 0.132,
 0.118, .118035,
T_DCF3= .0072764, 0.00336, 0.00336, 0.00336, 1.320908E-03, 0.000548,
 0.000283, 0.000255, 2.687071E-04,
BIOFAC2=  100,  100,  100,  100,  250,  500,  60,  60,  60,
BIOFAC1=  300,  30,  30,  30,  50,  100,  10,  10,  10,
RTF2=  .0008,  .0001,  .0001,  .0001,  .001,  .0001,  .00034,
 .00034,  .00034,
RTF3=  .0003,  .000001,  .000001,  .000001,  .001,  .000005,
 .0006,  .0006,  .0006,
RTF1= .01,  .001,  .001,  .001,  .04,  .001,  .0025,  .0025,
 .0025,
SLPF1= 4.2095E-09, 6.25E-11, 6.25E-11, 6.25E-11, 8.486873E-06,
 8.19E-10, 2.52E-10, 4.99E-11, 1.136329E-07,
SLPF2= 3.0755E-08, 5.25E-08, 5.25E-08, 5.25E-08, 2.827099E-08,
 3.4E-08, 2.78E-08, 2.36E-08, 2.363071E-08,
SLPF3= 3.443E-09, 1.65E-10, 1.65E-10, 1.65E-10, 5.147499E-10,
```

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 1.19E-10, 9.55E-11, 8.66E-11, 1.206122E-10,
SLPF4= 2.65992E-09, 1.28E-10, 1.28E-10, 1.28E-10, 3.855359E-10,
 9.1E-11, 7.07E-11, 6.4E-11, 8.710845E-11,
SLPF5= 3.443E-09, 1.65E-10, 1.65E-10, 1.65E-10, 5.147499E-10,
 1.19E-10, 9.55E-11, 8.66E-11, 1.206122E-10,
T_SLPFRN=  1.8E-12,  1.9E-13,  3.7E-12,  3E-15,  6.2E-12,  3.9E-11,
 1.5E-11,  3.7E-11,
T_KFACTR= 760,  150,  570,  250,
&END
```

Title: Air Pathway Assessment for the INL Remote-Handled Low-Level Waste Disposal Project

ECAR No.: 1370 ECAR Rev. No.: 1 Project File No.: NA Date: 09/28/2011

Appendix E, Microsoft Excel File Worksheets

The following are copied cells from three worksheets from the "ECAR-1370 Excel File:"

1. **"Bnd Lyr and Henry's Constant"** - Boundary Layer and Henry's Law Calculations
2. "**Screening"** - Screening Calculations Using CAP88-PC Dose to Inventory Factors
3. **"EMSOFT Dose"** - Sample of Dose Calculations using EMSOFT Flux per Ci Results

"Bnd Lyr and Henry's Constant" - Boundary Layer and Henry's Law Calculations

Boundary Layer Thickness

Nuclide	Dair (m^2/s)	Schmit Num	Boundary Layer depth (m)	Dair (cm2/d)	Dw ater (cm2/s)	Dw ater (cm2/d)	11.6	Annual Avg w ind-speed (based on monthly avg in Dec and April and Mar, See pg 2-8 of ICDF PA) km/hr
C-14	1.53E-05	1.02E+00	4.22E-03	1.32E+04	1.55E-05	1.34E+00	3.22	Annual Avg Wind speed (m/s)
H-3	7.94E-05	5.29E+00	2.44E-03	6.86E+04	3.52E-05	3.04E+00	1.50E-05	kinematic viscocity of air (m^2/s)
I-129	8.71E-06	5.81E-01	5.09E-03	7.53E+03	9.06E-06	7.83E-01	0.091876	Friction velocoty (m/s)
							60	Subsurface Temperature (F)
							288.6	Subsurface temperature (K)

Henry's Law Constant

Nuclide	Inverse H (Sander 1999) (mol/L-atm)	Inverse H Denham 2010 (mol/atm-kg) Oxidation III	Inverse H Denham 2010 (mol/atm-kg) Condition A	Dimension less H, Sander	Non-Dim H Denham 2010 Oxidation III	Non-Dim H Denham 2010 Condition A
C-14		2.8	0.038		0.0150938	1.11217495
H-3 (HT)	7.80E-04			5.42E+01		
H-3 (HTO)		2.10E+03	2.10E+03		2.01E-05	2.01E-05
I-129 (I2)	3.3	1.30E+29	6.30E+14	0.012639	3.25E-31	6.71E-17
I-129 (I2)	1.1			0.038421		

Dair Reference - All values calculated using EPA diffusion coefficient calculator
http://w w w .epa.gov/athens/learn2model/part-tw o/onsite/estdiffusion-ext.html

Rad	Chem Form	Dair (cm2/s)	Notes
C-14	CO2	0.153	Average of WL, FSG, FSG/LaBas methods, 15 C, 1 atm
H-3	H2	0.794	Average of WL, FSG, FSG/LaBas methods, 15 C, 1 atm
I-129	I2	0.0871	FSG/LaBas Method, 15 C, 1 atm

Title: Air Pathway Assessment for the INL Remote-Handled Low-Level Waste Disposal Project

ECAR No.: 1370 ECAR Rev. No.: 1 Project File No.: NA Date: 09/28/2011

"Screening" - Screening Calculations Using CAP88-PC Dose to Inventory Factors

		Site Boundary Location				100-m Location			
Nuclide	Half Life (yrs)	Total Inventory (Ci)	Conversion Factor (mrem/yr)/(Ci/yr)[a]	Screening Dose (mrem/yr)	Dose < 1 mrem?	Total Inventory at 100 yrs (Ci)	Conversion Factor (mrem/yr)/(Ci/yr)[a]	Screening Dose (mrem/yr)	Dose < 1 mrem?
Ar-39	269	5.01E-02	2.2E-08	1.1E-09	Yes	0.0388	1.1E-04	4.4E-06	Yes
Ar-42	33	5.51E-12	None	NA	NA	6.74E-13	None	NA	NA
C-14	5,730	4.33E+02	2.0E-04	8.7E-02	Yes	428	1.3E+00	535	No
H-3	12.3	3.92E+03	1.5E-05	5.9E-02	Yes	14.0	8.1E-02	1.13	No
I-129	1.57E+07	1.33E-01	4.7E-03	6.3E-04	Yes	0.133	2.4E+01	3.21	No
Kr-81	21,000	4.51E-12	4.7E-08	2.1E-19	Yes	4.49E-12	2.4E-04	1.1E-15	Yes
Kr-85	10.7	2.64E+02	4.6E-08	1.2E-05	Yes	0.411	2.4E-04	9.7E-05	Yes

a. Conversion Factors from CAP88-PC air dispersion modeling

"EMSOFT Dose" - Sample of Dose Calculations using EMSOFT Results

	Flux per Unit Conc from EMSOFT			Activated Metal Release			Misc Waste Release (EMSOFT)			Combined Metal and Non-Metal Dose			
Time (CY)	C-14 Unit Flux (mg/d/cm^2) per (mg/kg)	H-3 Unit Flux (mg/d/cm^2) per (mg/kg)	I-129 Unit Flux (mg/d/cm^2) per (mg/kg)	C-14 Act. Metal Release (Ci/yr)	H-3 Act. Metal Release (Ci/yr)	I-129 Act. Metal Release (Ci/yr)	C-14 Non-Metal Release (Ci/yr)	H-3 Non-Metal Release (Ci/yr)	I-129 Non-Metal Release (Ci/yr)	C-14 Dose (mrem/yr)	H-3 Dose (mrem/yr)	I-129 Dose (mrem/yr)	Total Dose (mrem/yr)
2068.3	3.8E-04	6.6E-04	2.7E-05	2.2E-04	2.2E-03	7.8E-12	7.4E+00	2.2E+00	1.2E-03	1.5E-03	3.3E-05	5.7E-06	1.5E-03
2068.4	3.8E-04	4.0E-04	4.8E-05	2.2E-04	2.2E-03	7.8E-12	7.5E+00	1.3E+00	2.1E-03	1.5E-03	2.0E-05	1.0E-05	1.5E-03
2068.5	3.7E-04	2.7E-04	6.3E-05	2.2E-04	2.2E-03	7.8E-12	7.3E+00	8.9E-01	2.8E-03	1.5E-03	1.3E-05	1.3E-05	1.5E-03
2068.6	3.6E-04	2.0E-04	7.4E-05	2.2E-04	2.2E-03	7.8E-12	7.0E+00	6.5E-01	3.3E-03	1.4E-03	9.8E-06	1.5E-05	1.4E-03
2068.7	3.5E-04	1.5E-04	8.1E-05	2.2E-04	2.2E-03	7.8E-12	6.8E+00	5.0E-01	3.6E-03	1.4E-03	7.6E-06	1.7E-05	1.4E-03
2068.8	3.3E-04	1.2E-04	8.6E-05	2.2E-04	2.2E-03	7.8E-12	6.5E+00	4.0E-01	3.8E-03	1.3E-03	6.1E-06	1.8E-05	1.3E-03

... Entire worksheet not copied due to size (see original electronic file)

2267.5	8.9E-07	3.9E-13	1.7E-06	2.1E-04	3.0E-08	7.8E-12	1.7E-02	1.3E-09	7.8E-05	2.2E-02	2.5E-09	1.9E-03	2.4E-02
2267.6	8.9E-07	3.9E-13	1.7E-06	2.1E-04	3.0E-08	7.8E-12	1.7E-02	1.3E-09	7.8E-05	2.2E-02	2.5E-09	1.9E-03	2.4E-02
2267.7	8.9E-07	3.9E-13	1.7E-06	2.1E-04	3.0E-08	7.8E-12	1.7E-02	1.3E-09	7.8E-05	2.2E-02	2.5E-09	1.9E-03	2.4E-02
2267.8	8.9E-07	3.8E-13	1.7E-06	2.1E-04	2.9E-08	7.8E-12	1.7E-02	1.3E-09	7.8E-05	2.2E-02	2.5E-09	1.9E-03	2.4E-02
2267.9	8.9E-07	3.8E-13	1.7E-06	2.1E-04	2.9E-08	7.8E-12	1.7E-02	1.3E-09	7.8E-05	2.2E-02	2.5E-09	1.9E-03	2.4E-02

Property	C-14	H-3	I-129	
Misc Waste Inv (Ci)	58.5	9.84	0.133	
Activated Met Inv (Ci)	374	3.91E+03	1.33E-05	
Half Life	5730	12.3	15700000	
Decay const (1/yr)	1.21E-04	5.64E-02	4.41E-08	
Corrosion RC (1/yr)	5.83E-07	5.83E-07	5.83E-07	
Misc Waste Conc (Ci/kg)	1.74E-06	3.68E-07	5.07E-09	
Unit Dose SB (mrem/Ci)	2.00E-04	1.50E-05	4.70E-03	Conversion Factors for Site Boundary receptor from CAP88-PC modeling
Unit Dose 100 m (mrem/Ci)	1.25	8.09E-02	24.1	Conversion Factors for 100-m receptor from CAP88-PC modeling
Bulk density (kg/m3)	1820	1820	1820	