

United States Department of Energy

Savannah River Site

**Vadose Zone Contaminant Migration Model - Multi-Layered
Software© (VZCOMML) Calculation Note and
Documentation**

January 4, 2007

**Prepared by:
Washington Savannah River Company, LLC
Savannah River Site
Aiken, SC 29808**



CONTACTS

Gregory G. Rucker - Author

Washington Savannah River Company
730-4B, Room 3043
Aiken, South Carolina 29808
803-952-6683
<mailto:gregory.rucker@srs.gov>

For a demonstration copy or more information about purchasing a copy of this software or selling the software yourself please contact:

John Olschon
Washington Savannah River Company
Technology Transfer and Business
773-41A, Rm. 239
Aiken, South Carolina 29808
803-725-8125
<mailto:john.olschon@srnl.doe.gov>

OSR 45-24# (Rev 5-19-2003)

Calculation Cover Sheet

| | | | | | |
|--|---|--|---|--|-------------|
| Project Modification of Vadose Zone Contaminant Migration Analysis Software | | Calculation Number Q-CLC-G-00068, Rev. 0 | | Project Number N/A | |
| Title Modification of Vadose Zone Contaminant Migration Analysis Software Vadose Zone Contaminant Migration Multi-Layer Model (VZCOMML) (U) | | Functional Classification GS | | Sheet 2 of 44 | |
| | | Discipline E&CSD | | | |
| Calc Level <input type="checkbox"/> Type 1 <input checked="" type="checkbox"/> Type 2 | | Type 1 Calc Status Preliminary <input type="checkbox"/> Confirmed <input type="checkbox"/> | | | |
| Computer Program No. Excel 2000 <input type="checkbox"/> N/A | | Version/Release No. VZCOMML V3.0 | | | |
| Purpose and Objective This calc-note is written to verify the calculations performed by the upgraded software program Vadose Zone Contaminant Migration Multi-Layer Model (VZCOMML), Version 3.0. This calculation note only addresses upgrades installed in the model since K-CLC-G-00051 (1999) and Q-CLC-B-00002 (1999). The model is an executable Excel 2000 workbook that is a one-dimensional, steady-state, vadose zone contaminant fate and transport model. The upgrades augment the software with more robust computational methods (less conservative) than in the original version. Specifically, the upgrades enhance the method used to calculate the retardation coefficient in the vadose zone and equilibrium partitioning equations used to estimate groundwater concentrations and soil screening levels. The soil screening module has been enhanced to screen for the presence of non-aqueous phase liquids (NAPLs) in soils. The output for the pore-water velocity module has been enhanced reporting of soil layers, soil moisture content, layer thickness, travel time, and pore-water velocity for each soil layer as well as either the weighted average and total values. Source layer water-filled and air-filled porosity is reported so users and reviewers will now be able to refer to the values used in the calculations. The former transport evaluation time (1000 years) was static and imbedded in the original code. The transport evaluation time has now been converted to a variable input and is user defined to increase the flexibility of the software. | | | | | |
| Summary of Conclusion The model calculates important contaminant transport parameters for any analyte on the TAL/TCL List plus a radionuclide suite. The parameters of greatest relevance are the mean time of travel through the vadose zone, the groundwater concentration, $SSL_{T/2}$ and MLSSL. The model is more consistent by using more compatible computation methods for flow in the vadose zone. Addition of complete equilibrium partitioning equations make these outputs more robust (less conservative) than in previous versions. Results for Version 3.0 will be significantly different than results from previous versions of the software and are not comparable due to computational changes within the software. | | | | | |
| Revisions | | | | | |
| Rev No. | Revision Description | | | | |
| 0 | Original Issue | | | | |
| Sign Off | | | | | |
| Rev No. | Originator (Print) Sign / Date | Verification / Checking Method | Verifier / Checker (Print) Sign / Date | Manager (Print) Sign / Date | |
| 0 | Gregory G. Rucker | | Kevin Brewer | Thomas Gaughan | |
| Design Agency - (Print) | | | Signature | | Date |
| Release to Outside Agency - (Print) | | | Signature | | Date |
| Security Classification of the Calculation | | | | | |

TABLE OF CONTENTS

| | |
|--|-----------|
| LIST OF TABLES | 4 |
| 1.0 INTRODUCTION..... | 5 |
| 1.1 Review of Model Basics | 5 |
| 1.2 Enhancements to VZCOMML | 6 |
| 2.0 ASSUMPTIONS..... | 9 |
| 3.0 INPUTS..... | 13 |
| 4.0 ANALYTICAL METHODS AND CALCULATIONS | 15 |
| 4.1 Estimation of Mixing Zone..... | 15 |
| 4.2 Dilution Attenuation Factor..... | 16 |
| 4.3 Derivation of Groundwater Concentrations | 16 |
| 4.4 Mean Travel Time in Groundwater | 20 |
| 4.5 Derivation of Retardation Coefficient..... | 22 |
| 4.6 Calculation of K_d for Organic Compounds | 24 |
| 4.7 Derivation of the Soil Screening Levels and Decay Adjusted Soil Screening Levels..... | 24 |
| 4.8 Calculation of the MLSSL | 28 |
| 5.0 RESULTS | 32 |
| 6.0 CONCLUSIONS | 33 |
| 7.0 REFERENCES..... | 35 |
| 8.0 ATTACHMENTS | 37 |

LIST OF TABLES

| | | |
|-------------|--|----|
| TABLE 3-1. | MODEL INPUT VARIABLES FOR MIXING ZONE AND DILUTION FACTOR E-7 TEST RUN | 13 |
| TABLE 3-2. | INPUT PARAMETERS FOR LAYER #1 FOR PORE-WATER VELOCITY E-7 TEST RUN | 13 |
| TABLE 3-3. | INPUT PARAMETERS FOR LAYER #2 FOR PORE-WATER VELOCITY E-7 TEST RUN | 13 |
| TABLE 3-4. | INPUT PARAMETERS FOR LAYER #3 FOR PORE-WATER VELOCITY E-7 TEST RUN | 14 |
| TABLE 3-5. | INPUT PARAMETERS FOR LAYER #4 FOR PORE-WATER VELOCITY E-7 TEST RUN | 14 |
| TABLE 3-5B. | SOURCE LAYER INPUT PARAMETERS | 14 |
| TABLE 3-6. | GEOTECHNICAL PARAMETERS FOR E-7 TEST RUN | 14 |
| TABLE 3-7. | CHEMICAL-SPECIFIC PARAMETERS FOR TRICHLOROETHYLENE E-7 TEST RUN... | 15 |
| TABLE 3-8. | CHEMICAL-SPECIFIC PARAMETERS FOR TECHNETIUM-99 E-7 TEST RUN..... | 15 |
| TABLE 4-1. | MIXING ZONE DEPTH PARAMETERS | 16 |
| TABLE 4-2. | DILUTION FACTOR PARAMETERS | 16 |
| TABLE 4-3. | GROUNDWATER EQUILIBRIUM/PARTITIONING EQUATION PARAMETERS..... | 17 |
| TABLE 4-4. | BIODEGRADATION/RADIOLOGICAL DECAY PARAMETERS | 18 |
| TABLE 4-5. | PARAMETERS FOR THE MEAN TIME OF MAXIMUM CONCENTRATION IN GROUNDWATER | 20 |
| TABLE 4-6. | PARAMETERS FOR CALCULATION OF SOIL-WATER VELOCITY | 21 |
| TABLE 4-7. | PARAMETERS FOR RETARDATION COEFFICIENT | 23 |
| TABLE 4-8. | PARAMETERS FOR SSL AND $SSL_{T1/2}$ EQUATIONS FOR METAL ANALYTES | 25 |
| TABLE 4-9. | PARAMETERS FOR SSL AND $SSL_{T1/2}$ EQUATIONS FOR MERCURY | 26 |
| TABLE 4-10. | PARAMETERS FOR $SSL_{T1/2}$ EQUATION FOR RADIONUCLIDES | 26 |
| TABLE 4-11. | PARAMETERS FOR $SSL_{T1/2}$ EQUATION FOR ORGANICS..... | 27 |
| TABLE 4-12. | PARAMETERS FOR MLSSL EQUATION FOR ORGANICS, INORGANICS AND METALS | 28 |
| TABLE 4-13. | PARAMETERS FOR DECAY ADJUSTED MLSSL EQUATION FOR RADIONUCLIDES .. | 28 |
| TABLE 4-14. | SUMMARY OF SCREENING DECISION LOGIC | 30 |
| TABLE 5-1. | OUTPUT FROM VZCOMML, V3 FOR E-7 TEST RUN..... | 33 |

1.0 INTRODUCTION

1.1 Review of Model Basics

This calc-note has been developed to verify calculations performed by the software program VZCOMML, Version 3.0, an executable Excel[®] 2000 workbook that is a one-dimensional, steady-state, vadose zone contaminant fate and transport model. The model was designed to meet four objectives: 1) to be utilized as a detailed waste-unit specific model for contaminant fate and transport analysis required under the Comprehensive Environmental Response Compensation/Liability Act (CERCLA) process; 2) to perform vadose zone contaminant fate and transport analysis in a manner that complies with the protocols specified by U.S. Environmental Protection Agency (USEPA), Region IV, South Carolina Department of Health and Environmental Control (SCDHEC), and the United States Department of Energy (USDOE); 3) to calculate site-specific soil screening levels (SSLs)/remedial goal objectives (RGOs); and 4) to evaluate the effectiveness of remedial alternatives by allowing the user to modify infiltration rates and hydraulic parameters that influence contaminant transport time and concentration. The method used in the model is consistent with the contaminant migration protocol of the Federal Facility Implementation Management Plan and USEPA Soil Screening Guidance (USEPA 1996). The input data, analytical equations, and model results are discussed in the following sections. The model estimates 1) the mean travel time in the vadose zone for any analyte (193 analytes in total) on the target analyte list (TAL), target compound list (TCL), or radionuclide list (RL) to arrive at the base of the vadose zone; 2) the maximum groundwater concentration at a receptor location on the edge of the waste unit; and 3) the maximum contaminant concentrations in soil that will not exceed the maximum contaminant level (MCL from the Safe Drinking Water Act) in groundwater.

The model is a combination of independent analytical modules whose outputs are linked to logic arguments and numerical outputs of all the other modules. There are four distinct modules. The dilution attenuation factor (DAF) and mixing zone are calculated using analytical equations programmed into a spreadsheet module called the "Soil

Screening Calculator”© (Rucker 1996). The pore water velocity module calculates pore-water velocity, soil moisture content, air-filled porosity, water-filled porosity, and travel times through a multi-layer soil column. The hydrogeological characteristics, including hydraulic conductivity, thickness, total porosity, and effective porosity, are user-defined for up to four homogenous layers and assembled into a heterogeneous soil column. The screening module automatically screens total contaminant concentrations from the waste unit source area against two calculated SSLs and a soil saturation limit (C_{sat}) value for each analyte and reports analytes that exceed these important limits.

The result module is the most sophisticated component of the model. It evaluates three fundamental logic criteria established in the Federal Facility Agreement (FFA) protocols for contaminant migration analysis. The criteria include 1) comparison of the calculated groundwater concentration to the action limit, 2) comparison of the retarded, mean travel time of a contaminant to reach the aquifer to the user-defined transport evaluation time, and 3) comparison of the unit source total contaminant concentrations to the mass limited soil screening limit (MLSSL). This module also computes the retardation coefficient, retarded, mean travel time for each analyte, and groundwater concentration for each analyte. The result module contains the action level [MCL from the Safe Drinking Water Act or preliminary remediation goal (PRG) from USEPA, Region IX] and will screen the estimated groundwater concentration for each analyte against its respective action level (among others as mentioned above), then automatically list all analytes that fail the screening. Finally, the result module calculates three different types of SSLs, the half-life SSL ($SSL_{T1/2}$), the MLSSL, and the default SSL. The SSLs are suitable for use as RGOs. Calculations are simultaneous for all 193 analytes if the appropriate input is provided.

1.2 Enhancements to VZCOMML

VZCOMML was first copyrighted in 1998 (SRS-98-530C). The original program was Version 1.0. Version 1.0 was modified one year later to incorporate an improved soil-pore water velocity module. This enhancement received a second copyright in 1999 and

is Version 2.0, the previous version (SRS-99-513C). The fundamental vision behind the design of Versions 1.0 and 2.0 was to provide a practical, consistent, easy-to-use, easy-to-understand, one-step model to implement the Federal Facility Agreement (FFA) protocols and to produce less conservative results than were generated by the USEPA SSL method. The final product would be acceptable to the regulators and conform to USEPA's soil screening guidance (USEPA 1996). The model would require only minimal data input with common, easily measured geotechnical parameters. Since VZCOMML did not have to solve the Richards, Phillips, or Green-Ampt infiltration equations, etc., it did not require exotic or esoteric experimental input parameters such as bubble pressure, disconnectedness index, suction front head, saturated suction, Green-Ampt wetting front suction, or sorptivity. VZCOMML has sought to avoid the superfluous pursuit of an academic exercise for contaminant migration evaluation and has been largely successful at doing so.

To accomplish its design objectives, Versions 1.0 and 2.0 used a number of computational expediencies which were incorporated into the program code. As an example, the original code used the saturated zone form of the retardation coefficient equation instead of the unsaturated zone form of the equation. The reasoning behind this was simple. It was easier to calculate the saturated form of the retardation equation because the saturated equation required three parameters to calculate. This can be contrasted to the unsaturated form which required those three parameters, plus a computational subroutine, plus five more parameters that required tabled values to determine the input. The only difference in the final values was a slightly more conservative result (most of the time +/-20% of the moisture content), which, at the time of software development, was considered a positive feature due to regulatory concerns.

Because VZCOMML has been in continuous use for over six years and is being commercially marketed, it has been subjected to numerous in-house and national-level critiques, peer reviews, and improvement suggestions. The following modifications have been incorporated into the new Version 3.0:

1. Saturated zone form of the retardation coefficient equation was replaced by the unsaturated zone form of the retardation equation using an effective moisture content term. This makes the retardation compatible with the manner of calculation of pore-water velocity and mimics the physical behavior of the water content and suction in the unsaturated zone.
2. All the equilibrium equations have been upgraded to account for complete partitioning into vapor, aqueous and sorbed phases. This means that total contaminant concentrations should now be used as the primary input parameter rather than converting from a total concentration to a sorbed-phase concentration. This change applies to all the partitioning equations included in the model, including the SSL equations. Additionally, equilibrium calculations are made to relate to Source Layer moisture and air-filled porosity.
3. The transport evaluation time (T_e) has been changed from a fixed value embedded into the code to a user-defined variable. Users can now adjust the evaluation time to suit the contaminant and site-specific conditions and are no longer limited to a static 1,000 year evaluation time.
4. A C_{sat} screening step has been incorporated into the software. This is a new feature designed to determine the presence of non-aqueous phase liquid (NAPL) for organic contaminants in soil samples. This feature calculates a C_{sat} value and logic screening test for each organic analyte.
5. The configuration of the soil-pore water velocity module has been enhanced to display more detailed information about the structure of the soil column. The soil column now begins with a Source Layer. The Source Layer is the upper most in a sequence of four other homogeneous soil layers that in total represent a single heterogeneous soil column beneath the source. The Source Layer and its geotechnical parameters are not used in the transport equations. Additionally, the manner of inputting the “K” and “b” parameters has been modified to limit inputs

to the tabled values only since these are fitted values and this has been a point of confusion over the years. The output includes summary data for total and effective porosities as well as air and water-filled porosities and effective moisture content. This module will now alert the user if the infiltration rate exceeds any layer's hydraulic conductivity, a situation not defined by the model and synonymous with ponded/perched water.

6. A decay term has been added to the Mass Limit Soil Screening Level for radionuclides only since this is the probable state of nature.
7. An independent spreadsheet was added (Custom Analyte) to determine concentrations, transport time, and SSLs for analytes not found on any of the other spreadsheets. The spreadsheet uses the dilution factor, geotechnical values, evaluation time and pore-water velocity from other modules in the model.
8. Mercury equilibrium equations have been improved to include soil, liquid and vapor phases.

2.0 ASSUMPTIONS

The calculations simulate dispersive mixing in the saturated zone, and equilibrium partitioning in the vadose zone. Transport time in the vadose zone is determined by Darcy's Law and represents mean flow. A homogeneously distributed and infinite source of contaminants is conservatively assumed in the source layer to simplify leaching estimates. Dispersion is not incorporated into the vadose zone transport estimate. Reversible linear soil-water distribution of contaminants at equilibrium is represented in the source zone by the distribution coefficient (K_d) and Henry's Law Constant (H'), which is calculated according to USEPA soil screening guidance (USEPA 1996) for organic contaminants and a tabled value for mercury. The organic compound distribution coefficients used in the model are estimated from the organic carbon fraction (K_{oc}) described by USEPA. The model can use either the USEPA default value for soil organic carbon fraction (f_{oc}) of 0.002 or the unit-specific organic carbon fraction where

total organic carbon analyses have been performed (preferably EPA Method 9060) near waste unit soils. K_{ds} for metals and radionuclides were selected from Savannah River Site (SRS) specific leaching studies or scientific literature. These K_d values may need to be adjusted by the user depending on the known conditions at the waste site under investigation.

The default K_{ds} loaded in the spreadsheet model are both site-specific and calculated. The K_{ds} for organic analytes are calculated from their respective chemical-specific K_{oc} s and f_{oc} s. The source of the K_{oc} values used in the calculations came from two primary sources: 1) USEPA, *Technical Background Document for Soil Screening Guidance* (USEPA 1996) and 2) *Electronic Handbook of Risk Assessment Values*, Volume 6, Issue 1/2, (c) Electronic Handbook Publishers, Inc. (ERAV 1997). The K_{ds} for metal and radionuclide analytes are site-specific and were selected from several sources, including the following: 1) *Technical Background Document for Soil Screening Guidance* (USEPA 1996) and 2) *Estimation of Geochemical Parameters for Assessing Subsurface Transport at the Savannah River Plant* (Looney et al. 1987), 3) *Appropriate K_d Values for SCDF Project Including C-14 and Np-237*, (Denham 1996), and 4) "Default Soil Solid/Liquid Partition Coefficients, K_{ds} for Four Major Soil Types: A Compendium," *Health Physics* (Sheppard and Thibault 1990). The site-specific K_d selections from the literature were made to best match conservative the geochemical conditions (sandy soil) present at SRS and so should be representative.

First order decay of organic and radiological analytes is incorporated into the calculations utilizing published environmental half-lives for biological reactions and no daughter-in-growth is considered for either organic or radiological analytes. Environmental half-life values are available for organic compounds in various media. The environmental half-lives chosen for this study are the aerobic values reported for soil media.

Radiological half-lives were selected from *Electronic Handbook of Risk Assessment Values* (ERAV 1997). Biological half-lives were selected from *Handbook of Environmental Degradation Rates* (Howard 1991).

Several caveats should be noted with regard to user-definable variables. Even though degradation half-lives for organic analytes are included in the software, they serve as placeholders for calculating rate constants to illustrate the power of the software and are not necessarily default values. The use of a degradation rate for any organic analyte has always been optional in the software, and its inclusion does not mean it is appropriate or a preferred value. Degradation half-lives are a user-definable variable on the input sheets in the software, i.e., the user determines the appropriateness and/or magnitude of degradation depending upon site-specific characterization data and the user defends those values accordingly.

The software has always contained a feature that will cancel the time-decay/degradation calculations for any organic or radioactive analyte. If the value, 1.0E+99, is substituted for the half-life, the use of the time-decay feature in the software is disabled. When the time-decay feature is disabled, the $SSL_{T1/2}$ will calculate an identical value as the default SSL. This feature should not be actuated for any radiological analyte. The user is responsible to review all the chemical-specific and user-defined variables, which include the distribution coefficient, octanol-water partitioning coefficient, Henry's Law Constant, aqueous solubility limit, bulk density, hydraulics, and f_{oc} , for appropriateness and applicability based upon characterization knowledge. While the variables included in the software represent best estimates for SRS conditions, the user is still under obligation to review and validate the use of these values in their own analysis. The software author is not obligated to justify any of the variables used in anyone else's analysis.

The average total soil concentrations should be used for user supplied site-specific concentrations of soil analytes subject to leaching (not reasonable maximum exposure concentrations). The pH of the pore water is assumed to be approximately 6.0 for default parameters. Maximum analytical concentrations of samples may be used to calculate bounding SSL values and screening for levels for NAPLs. Hot spots may be modeled if consistent with the unit-specific conceptual site model (CSM). The following major assumptions are used in the model:

- The source is considered to be infinite except for mass-balanced calculations.
- The system is at equilibrium with respect to adsorption.
- Contaminants are homogeneously distributed in the vadose zone.
- Adsorption is linear with concentration.
- Contaminant adsorption to soil is reversible.

3.0 INPUTS

Only the model outputs affected by the upgrades will be evaluated in this calculation note. The DAF and mixing zone module will be calibrated to the initial calculation note

parameters, K-CLC-G-00051. For the purpose of this calc-note, the following parameters will be provided so that the model output can be verified and hand checked.

Table 3-1. Model Input Variables for Mixing Zone and Dilution Factor E-7 Test Run

| Parameter | Definition | Value | Unit | Reference |
|----------------|--|-------|-----------|---------------|
| L | Source length parallel to groundwater flow | 60 | Feet | Unit-specific |
| I | Vertical infiltration rate through vadose zone | 1.25 | Feet/year | Flack et al |
| K | Saturated horizontal hydraulic conductivity | 1449 | Feet/year | Unit-specific |
| d _a | Aquifer thickness | 100 | Feet | Unit-specific |
| i | Horizontal hydraulic gradient | .009 | Feet/feet | Unit-specific |

The calibrated DAF from K-CLC-G-00051 is 3.08. This value should be used for the DAF when hand calculations are performed for checking purposes.

Table 3-2. Input Parameters for Layer #1 for Pore-Water Velocity E-7 Test Run

| Parameter | Definition (sandy clay loam) | Value | Unit | Reference |
|-----------------|------------------------------|-------|---------------|------------------|
| Th ₁ | Thickness layer 1 | 10 | Feet | Unit-specific |
| b ₁ | “b” parameter layer 1 | 7.12 | Dimensionless | Clapp&Hornberger |
| n _{e1} | Effective porosity layer 1 | 0.30 | Fraction | Looney et al. |
| n _{T1} | Total porosity layer 1 | 0.40 | Fraction | Looney et al. |
| K _{s1} | K parameter layer 1 | 131.0 | Feet/Year | Clapp&Hornberger |

Table 3-3. Input Parameters for Layer #2 for Pore-Water Velocity E-7 Test Run

| Parameter | Definition (clay) | Value | Unit | Reference |
|-----------------|----------------------------|-------|---------------|------------------|
| Th ₂ | Thickness layer 2 | 50 | Feet | Unit-specific |
| b ₂ | “b” parameter layer 2 | 11.4 | Dimensionless | Clapp&Hornberger |
| n _{e2} | Effective porosity layer 2 | 0.25 | Fraction | Looney et al. |
| n _{T2} | Total porosity layer 2 | 0.40 | Fraction | Looney et al. |
| K _{s2} | K parameter layer 2 | 16.0 | Feet/Year | Clapp&Hornberger |

Table 3-4. Input Parameters for Layer #3 for Pore-Water Velocity E-7 Test Run

| Parameter | Definition (loamy sand) | Value | Unit | Reference |
|-----------------|-------------------------|-------|---------------|------------------|
| Th ₃ | Thickness layer 3 | 10 | Feet | Unit-specific |
| b ₃ | “b” parameter layer 3 | 4.38 | Dimensionless | Clapp&Hornberger |

| | | | | |
|----------|----------------------------|--------|-----------|------------------|
| n_{e3} | Effective porosity layer 3 | 0.22 | Fraction | Looney et al. |
| n_{T3} | Total porosity layer 3 | 0.40 | Fraction | Looney et al. |
| K_{s3} | K parameter layer 3 | 1772.0 | Feet/Year | Clapp&Hornberger |

Table 3-5. Input Parameters for Layer #4 for Pore-Water Velocity E-7 Test Run

| Parameter | Definition (silty clay loam) | Value | Unit | Reference |
|-----------|------------------------------|-------|---------------|------------------|
| Th_4 | Thickness layer 4 | 10 | Feet | Unit-specific |
| b_4 | “b” parameter layer 4 | 7.75 | Dimensionless | Clapp&Hornberger |
| n_{e4} | Effective porosity layer 4 | 0.25 | Fraction | Looney et al. |
| n_{T4} | Total porosity layer 4 | 0.44 | Fraction | Looney et al. |
| K_{s4} | K parameter layer 4 | 43 | Feet/Year | Clapp&Hornberger |

Table 3-5b. Source Layer Input Parameters

| Parameter | Definition (clay) | Value | Unit | Reference |
|-----------|---------------------------------|-------|---------------|------------------|
| Th_s | Thickness source layer | 7 | Feet | Unit-specific |
| b_s | “b” parameter source layer | 11.4 | Dimensionless | Clapp&Hornberger |
| n_{es} | Effective porosity source layer | 0.30 | Fraction | Looney et al. |
| n_{Ts} | Total porosity source layer | 0.40 | Fraction | Looney et al. |
| K_{Ss} | K parameter source layer | 16 | Feet/Year | Clapp&Hornberger |

Hydraulic conductivity (from Table 1 in the model) is now referred to as the “K” parameter to reduce confusion with actual unfitted hydraulic conductivity values.

Table 3-6. Geotechnical Parameters for E-7 Test Run

| Parameter | Definition | Value | Unit | Reference |
|--------------|-------------------------------------|-------|-----------------|----------------|
| d_s | Vertical thickness of source | 7.0 | Feet | Unit-specific |
| ED | Exposure duration | 70.0 | Years | USEPA |
| L_v | Depth to groundwater $\Sigma(Th_i)$ | 80.0 | Feet | Calculated |
| T_e | Evaluation Time | 1000 | Years | User selection |
| ρ_β | Dry soil bulk density | 1.7 | Kilograms/liter | Unit-specific |
| f_{oc} | Fraction organic carbon | 0.003 | Fraction | Unit-specific |

Table 3-7. Chemical-Specific Parameters for Trichloroethylene E-7 Test Run

| Parameter | Definition | Value | Unit | Reference |
|------------------|----------------------------|--------|-----------------|----------------|
| K _{oc} | Organic carbon coefficient | 265 | Liters/kilogram | ERAV |
| T _{1/2} | Degradation half-life | 10.0 | Years | Howard, et. al |
| C _t | Total soil concentration | 5.0 | mg/kg | Unit-Specific |
| C _w | MCL | 5.0 | µg/L | SDWA |
| S | Aqueous solubility limit | 1100.0 | mg/L | USEPA |
| H | Henry's Law Constant | 0.422 | Unitless | USEPA |

Table 3-8. Chemical-Specific Parameters for Technetium-99 E-7 Test Run

| Parameter | Definition | Value | Unit | Reference |
|------------------|----------------------------------|---------|-------|--------------------|
| K _{oc} | Organic carbon coefficient | NA | NA | NA |
| K _d | Soil-water partition coefficient | 0.1 | L/kg | Looney et al. 1987 |
| T _{1/2} | Radiological decay half-life | 217,000 | Years | ERAV |
| C _t | Total soil concentration | 1.0 | pCi/g | Unit-Specific |
| C _w | MCL | 900 | pCi/L | SDWA |

4.0 ANALYTICAL METHODS AND CALCULATIONS

All significant calculations performed by the software are included in Section 4.0. The Version 3.0 enhancements contain additional notes of explanation.

4.1 Estimation of Mixing Zone

Table 4-1 lists the parameters and definitions for estimating the mixing zone. The mixing zone depth (d) is estimated by the following mixing zone equation:

$$d = (0.0112 \cdot L^2)^{0.5} + d_a \cdot (1 - e^{((-L \cdot 1)/K \cdot i \cdot d_a)}) \quad (1)$$

where:

Table 4-1. Mixing Zone Depth Parameters

| Parameter | Definition | Units |
|-----------|------------|-------|
|-----------|------------|-------|

| | | |
|----------------|--|------------------|
| d | Mixing zone depth (or actual depth of MZ) | Calculated, feet |
| K | Saturated horizontal hydraulic conductivity | Feet/year |
| i | Horizontal hydraulic gradient | Feet/feet |
| I | Vertical infiltration rate through vadose zone | Feet/year |
| d _a | Aquifer thickness | Feet |
| L | Length of source parallel to groundwater flow | Feet |

4.2 Dilution Attenuation Factor

Table 4-2 lists the terms and definitions for deriving the DAF. The DAF is estimated by the following equation:

$$DAF = 1 + \frac{K \cdot i \cdot d}{I \cdot L} \quad (2)$$

where:

Table 4-2. Dilution Factor Parameters

| Parameter | Definition | Units |
|-----------|--|----------------------|
| DAF | Dilution Attenuation Factor | Calculated, unitless |
| K | Saturated vertical hydraulic conductivity | Feet/year |
| g | Horizontal hydraulic gradient | Feet/feet |
| I | Vertical infiltration rate through vadose zone | Feet/year |
| d | Mixing zone depth | Calculated, feet |
| L | Length of source parallel to groundwater flow | Feet |

4.3 Derivation of Groundwater Concentrations

The following equations used to derive groundwater concentrations are enhancements in Version 3.0. These equations were not used in the earlier versions of VZCOMML; therefore and as a caveat, V3.0 results will not be comparable to V2.0 results. Earlier versions used the identical form of a truncated equilibrium equation to derive the groundwater concentrations for all classes (metals, volatile organic compounds (VOCs), semivolatile organic compounds (SVOCs), etc.) of analytes. In earlier versions, volatilization and liquid phases were ignored under the premise that their omission from the calculation would have a negligible impact on the result. This assumption made the result slightly more conservative than that achieved with a complete equilibrium equation and all analytes could be computed with one basic equation. Because three phase

equilibrium is now accounted for in the model, a variety of specific partitioning equations are now required. As in previous versions, all the equilibrated leachate concentrations are divided by the DAF due to dilution in the aquifer.

Groundwater equations used in Version 3.0 have been expanded to include the use of various but complete equilibrium equations to predict groundwater concentrations. The complete equilibrium equations now account for the total mass of contaminant present in a sample, including vapor (where appropriate), solid (sorbed), and aqueous phases. Therefore, mean total contaminant concentrations (C_t) are now used as input values.

The equations used in the model are all a form of a linear isotherm (exponent 1) based on the Freundlich equation. These contain the same basic equation used by USEPA in *Soil Screening Guidance*, USEPA/540/R-95/128, May 1996. The basic equilibrium partitioning equation for predicting a groundwater concentration for mercury is expressed as follows:

$$C_{gw} = \frac{C_t \cdot [1000 \text{ ug/mg}]}{\left(K_d + \frac{(\theta_w + H \cdot \theta_a)}{\rho_\beta} \right)} / (DAF) \quad (3a) \text{ where:}$$

Table 4-3. Groundwater Equilibrium/Partitioning Equation Parameters

| Parameter | Definition | Units |
|--------------|--|----------------------|
| DAF | Dilution Attenuation Factor | Calculated, unitless |
| C_t | Total Soil Concentration | mg/kg, pCi/g |
| C_{gw} | Concentration in groundwater at hypothetical well at edge of source area | μg/L, pCi/L |
| K_d | Distribution coefficient | L/kg |
| H | Henry's Law Constant for volatile organics/mercury | Unitless |
| θ_w | Source Zone water-filled soil porosity ($V_{\text{water}}/V_{\text{total}}$) | Percent/decimal |
| θ_a | Source Zone air-filled soil porosity ($V_{\text{air}}/V_{\text{total}}$) | Percent/decimal |
| ρ_β | Soil bulk density | kg/L |

Equation 3a is unique in the software to calculate the groundwater concentration for mercury, because mercury is the only metal on the TAL that exerts vapor pressure. In fact, the vapor pressure for mercury can be one to four orders of magnitude higher than the vapor pressure for some polychlorinated biphenyls (PCBs). The equation

incorporates partitioning to soil-pore air because of the vapor pressure. There will be mass, albeit small, in the vapor phase as a result.

A slightly different equilibrium partitioning equation that eliminates the air-filled porosity (vapor phase) term is used to calculate the groundwater concentration for the remainder of the TAL metals and radionuclides since none of these exert any vapor pressure, and there will be no contaminant mass in the vapor phase. Therefore, θ_a does not have to be included in the equation since all mass will be partitioned between liquid and sorbed phases only. The groundwater concentration equation for metals is expressed as follows:

$$C_{gw} = \frac{C_t \cdot [1000 \text{ ug/mg}]}{\left(K_d + \frac{\theta_w}{\rho_\beta} \right)} / (DAF) \quad (3b)$$

For radioactive analytes a first-order decay term and a different conversion factor is included and the groundwater equilibrium-partitioning equation is expressed as:

$$C_{gw} = \frac{\left(C_t \cdot [1000 \text{ g/kg}] \cdot e^{(-0.693 \cdot T_{Mean} / T_{1/2})} \right)}{\left(K_d + \frac{\theta_w}{\rho_\beta} \right)} / (DAF) \quad (3c)$$

Table 4-4. Biodegradation/Radiological Decay Parameters

| Parameter | Definition | Units |
|------------|--------------------------------------|-------|
| T_{Mean} | Mean Travel Time in vadose zone | Years |
| $T_{1/2}$ | Biological or Radiological half-life | Years |

Because the TAL metals do not degrade, no decay term is included in equation 3b based on the assumption that metal half-life is infinite. Equation 3c is similar to equation 3b, but accounts for radiological decay by using a simple first-order decay term that does not include daughter in-growth.

The final equilibrium partitioning equation used in the model is for organic analytes and is similar to equation 3c. Because all the organic analytes exert vapor pressure, albeit very low pressures for some compounds, partitioning to air-filled soil porosity is incorporated into the equation. The incorporation of the vapor phase will impact volatile groundwater contaminant concentrations more when compared with other low volatility analytes. Volatile contaminants have the highest vapor pressures (consequently a higher Henry's Law Constant) of all the analytical classes. The higher vapor pressures will partition more of the total contaminant mass into vapor phase, thereby lowering the mass to be distributed in groundwater. Additionally, since organic compounds can degrade by natural processes, the equation also includes a simple first order degradation term. The groundwater concentration equation for organic compounds is expressed below:

$$C_{gw} = \frac{(C_t \cdot e^{(-0.693 \cdot T_{Mean} / T_{1/2})})}{\left(K_d + \frac{(\theta_w + H \cdot \theta_a)}{\rho_\beta} \right)} / (DAF) \cdot [1000 \text{ ug/mg}] \quad (3d)$$

As noted in the above calculations, several conversion factors are necessary to maintain the correct dimensional units. All groundwater concentrations for metallic and organic analytes are reported in $\mu\text{g/L}$ in the model including the action levels. Since input total soil concentrations are in terms of mg/kg , the equations must include a conversion to μg to enable the comparison to an action level. Input total soil concentrations for radionuclides are in terms of pCi/g , and the groundwater concentration must be converted to pCi/L before it is compared to an action level.

The addition of a biological decay factor is a viable method and consistent with *Technical Background Document for Soil Screening Guidance* (USEPA 1996) and *Soil Screening Guidance for Radionuclides: Technical Background Document* (USEPA 2000). The SSLs are overly conservative with respect to SRS site-specific conditions, e.g., a thick unsaturated zone and layered soils of differing hydraulic conductivity. Some of the conservatism can be eliminated by estimating a mean travel time through the vadose zone (T_{Mean}) and then using this estimate to calculate the amount of decay as the

contaminant is being transported to the aquifer. The decay calculations augment the soil screening calculations resulting in a higher, but still protective SSL.

4.4 Mean Travel Time in Groundwater

T_{Mean} is the mean retarded contaminant travel time in the vadose zone. T_{Mean} is calculated by dividing the distance from the bottom of the contamination in the Source Layer to the top of the water table surface by the mean retarded pore water velocity using the following equation:

Travel Time Equation

$$T_{\text{mean}} = \frac{L_v \cdot R}{V_s} \quad (4)$$

where:

Table 4-5. Parameters for the Mean Time of Maximum Concentration in Groundwater

| Parameter | Definition | Units |
|-------------------|---|-----------------------|
| T_{mean} | Mean Travel Time to the top of the aquifer | Calculated, years |
| L_v | Distance from the bottom of source layer to the water table | Calculated, feet |
| V_s | Pore- water velocity in the vadose zone | Calculated, feet/year |
| R | Retardation coefficient | Calculated, unitless |

V_s is determined from the infiltration rate, total and effective porosity, and K parameter (saturated hydraulic conductivity) by the following series of equations:

$$V_s = \frac{I}{\theta_e} \quad (5a)$$

$$\theta_e = \theta_w \cdot \frac{n_e}{n_t} \quad (5b)$$

(5c)

where:

$$\theta_w = n_t \cdot \left(\frac{I}{K_s} \right)^{\left(\frac{1}{(2 \cdot b + 3)} \right)}$$

Table 4-6. Parameters for Calculation of Soil-Water Velocity

| Parameter | Definition | Units |
|------------|--|-----------|
| V_s | Soil-pore water velocity in vadose zone | Feet/year |
| I | Vertical infiltration rate through vadose zone | Feet/year |
| Θ_w | Volumetric moisture content ($V_{\text{water}}/V_{\text{soil}}$) | Fraction |
| Θ_e | Effective moisture content | Fraction |
| n_e | Effective porosity | Fraction |
| n_t | Total porosity | Fraction |
| b | Soil-specific exponential parameter | Unitless |
| K_s | K Parameter | Feet/year |

Equations 5a, 5b, and 5c represent the equations used by the software to calculate the pore water velocity in the vadose zone. Equation 5c is attributable to the work by Hornberger and Clapp and calculates the volumetric moisture content, θ or θ_w .

Darcy's Law for groundwater flow velocity in the saturated zone is defined as, $V_D = -K_s \cdot A \cdot i$. Darcy's equation describes groundwater movement in the saturated zone as the bulk flow of water through a cross-sectional area (A), under gradient (i), through a medium of both soil particles (solids) and through soil pores. This is also referred to as the Darcy velocity.

However, the Darcy velocity is not the same as the water velocity flowing through the soil pores (V_{gw}), because the equation does not consider that water does not flow through the entire cross-sectional area of soil strata. The macroscopic pore water velocity for the saturated zone is actually determined by dividing the Darcy velocity by the effective porosity or $V_{\text{gw}} = V_D/n_e$.

Darcy's Law can be extrapolated from the above for flow in the unsaturated (vadose) zone as well. It is expressed as $V_s = I/\theta_w$ (USEPA 1988 from Enfield et al. 1982). This equation implies steady-state conditions or those that can be assumed to be steady-state.

In equations 5a and 5c, the infiltration rate (I) is equivalent to the unsaturated hydraulic conductivity and is contrasted to (K_s), the saturated hydraulic conductivity and represents the ratio of available moisture. Because hydraulic conductivity in the vadose zone is a function of water content such that $K=K(\theta)$, pore water velocity is determined as the ratio of I and the volumetric water content of the soil, I/θ_w .

The percent of water content of the soil is the ratio between I (unsaturated hydraulic conductivity) and K_s (saturated hydraulic conductivity) multiplied by the available volume of pore space. The result is θ_w , the volumetric moisture content. As explained above for saturated conditions, recognizing that the entire cross-sectional area of soil pores does not support flow, the equation for pore-water velocity in the vadose zone (5a) becomes, $V_s=I/\theta_e$.

Equation 5b calculates the effective moisture content θ_e , which is a representation of the available porosity where soil-pore water can actually flow, thereby eliminating dead-end pore space or disconnected porosity. This term is interpreted to be the ratio of porosity which will actually facilitate flow through interconnected soil pores as opposed to a condition where soil pore spaces are disconnected.

The soil-pore water velocity is calculated in an independent module. Enhanced display of vadose zone parameters can be found in this module, including output for each soil layer including totals or weighted averages of values.

4.5 Derivation of Retardation Coefficient

The method for calculating retardation has been improved in Version 3.0 as explained earlier in this note. The equation in the earlier versions of VZCOMML was the saturated zone form of the retardation coefficient equation (Freeze and Cherry 1979). The enhanced version uses a soil physics-based calculation for unsaturated zone flow characteristics. The unsaturated form of the retardation coefficient equation is expressed as follows:

$$R = 1 + \frac{(K_d \cdot \rho_\beta)}{\theta_e} \quad (6)$$

where:

Table 4-7. Parameters for Retardation Coefficient

| Parameter | Definition | Units |
|--------------|-------------------------------------|----------|
| R | Unsaturated retardation coefficient | Unitless |
| K_d | Distribution coefficient | L/kg |
| ρ_β | Soil bulk density | kg/L |
| n_T | Total soil porosity | Fraction |
| θ_e | Effective moisture content | Percent |

Equations 5b, 5c and 6 reflect the actual equations the model uses to compute the retardation although it is being computed in several sequential steps in the model. The model calculates θ_w once, then uses the computed result to calculate both the soil-pore water velocity and retardation coefficient.

Equation 5b calculates the term " θ_e " (n_e/n_T) which can be referred to as the effective moisture content, as explained previously. Using the effective moisture content is a practical way to calculate contaminant retardation for unsaturated soils, since water content, along with hydraulic conductivity and infiltration, are some of the primary factors that determines flow in the vadose zone.

4.6 Calculation of K_d for Organic Compounds

The K_d of an organic compound is related to the organic-carbon partition coefficient (f_{oc}) through the following distribution coefficient equation:

$$K_d = f_{oc} \cdot K_{oc} \quad (7)$$

A default f_{oc} of 0.2% (.002) can be used as a conservative value if a unit-specific value is not available (USEPA 1996). A unit-specific f_{oc} value should be substituted if the organic carbon content of the soil has been analyzed. Chemical-specific K_{oc} values were obtained from the literature, and some were calculated using formulas relating the octanol-water partitioning coefficient or water solubilities to the K_{oc} .

4.7 Derivation of the Soil Screening Levels and Decay Adjusted Soil Screening Levels

Three types of SSLs are calculated for each analyte in the model. They are the default SSL, MLSSL, and the $SSL_{T1/2}$ (decay adjusted SSL).

The SSL can be the equivalent of a Remedial Goal Option (RGO) or Preliminary Remedial Goal (PRG) for contaminant migration COCs (contaminants of concern). These are referred to as the CM-RGO (contaminant migration RGO) or CM-PRG. The difference between the SSL and RGO/PRG, is that the RGO/PRG is selected for inclusion into a regulatory document as a compliance standard, which in effect, is a soil cleanup level. VZCOMML uses complete, linear equilibrium equations and any of the calculated SSLs could be used as a RGO/PRG. The user should evaluate the three types of SSLs and select the most appropriate value as the RGO/PRG. In almost every instance, the user should select the highest of the SSLs as the RGO/PRG.

The SSL equations are more robust because the calculations now include equilibrium-partitioning components for vapor, sorbed, and aqueous phases. Because of equilibrium partitioning, the total mass concentration (C_i) of the analyte should now be used for the

soil concentration input. Converting the total mass concentration to a sorbed concentration (C_s) is no longer required.

Due to the variety of chemical classes of analytes included in the model (organics, inorganics, volatile metal, and radionuclides), there is a greater variety of SSL equations. The greater variety of equations is needed to properly account for mass phase distribution based upon the physical properties of the analyte. The metals are the only class of analytes where degradation is assumed to have an infinite half-life. In the case of metals, both the default SSL and the $SSL_{T_{1/2}}$ are equal values. The SSL equation for any metal analyte (excluding mercury) is expressed as follows:

$$\text{Where: } SSL_{T_{1/2}} = \frac{MCL \cdot DAF \cdot \left(K_d + \frac{\theta_w}{\rho_\beta} \right)}{e^{(-0.693 \cdot T_{Mean} / T_{1/2})}} / [1000 \text{ ug/mg}] \quad (8a)$$

Table 4-8. Parameters for SSL and $SSL_{T_{1/2}}$ Equations for Metal Analytes

| Parameter | Definition | Units |
|-------------------------|---|----------|
| SSL and $SSL_{T_{1/2}}$ | Soil Screening Level | mg/kg |
| MCL | Maximum Contaminant Level, PRG | mg/L |
| DAF | Dilution Attenuation Factor | Unitless |
| K_d | Distribution coefficient | L/kg |
| ρ_β | Soil bulk density | Kg/L |
| θ_w | Volumetric moisture content | Percent |
| T_{Mean} | Mean travel time to top of aquifer | Years |
| $T^{1/2}$ | Degradation half-life (Assumed to be infinite for metals) | Years |

The MCL parameter is either the MCL or the PRG value.

The SSL equation for mercury (the only volatile metal analyte) is expressed as follows:

$$SSL_{T_{1/2}} = \frac{MCL \cdot DAF \cdot \left(K_d + \frac{(\theta_w + H \cdot \theta_a)}{\rho_\beta} \right)}{e^{(-0.693 \cdot T_{Mean} / T_{1/2})}} / [1000 \text{ ug/mg}] \quad (8b)$$

Where:

Table 4-9. Parameters for SSL and $SSL_{T_{1/2}}$ Equations for Mercury

| Parameter | Definition | Units |
|-------------------------|---|----------|
| SSL and $SSL_{T_{1/2}}$ | Soil Screening Level | mg/kg |
| MCL | Maximum Contaminant Level, PRG | mg/L |
| DAF | Dilution Attenuation Factor | Unitless |
| K_d | Distribution coefficient | L/kg |
| ρ_β | Soil bulk density | Kg/L |
| θ_w | Volumetric moisture content | Percent |
| T_{Mean} | Mean travel time to top of aquifer | Years |
| $T^{1/2}$ | Degradation half-life (Assumed to be infinite for metals) | Years |

The $SSL_{T_{1/2}}$ equation for radionuclides which includes first-order decay is expressed as:

$$SSL_{T_{1/2}} = \frac{MCL \cdot DAF \cdot [0.001 \text{ kg/g}] \cdot \left(K_d + \frac{\theta_w}{\rho_\beta} \right)}{e^{(-0.693 \cdot T_{Mean} / T_{1/2})}} \quad (8c)$$

Where:

Table 4-10. Parameters for $SSL_{T_{1/2}}$ Equation for Radionuclides

| Parameter | Definition | Units |
|-----------------|-------------------------------------|----------|
| $SSL_{T_{1/2}}$ | Decay Adjusted Soil Screening Level | pCi/g |
| MCL | Maximum Contaminant Level, PRG | pCi/L |
| DAF | Dilution Attenuation Factor | Unitless |
| K_d | Distribution coefficient | L/kg |
| ρ_β | Soil bulk density | Kg/L |
| θ_w | Volumetric moisture content | Percent |
| T_{Mean} | Mean travel time to top of aquifer | Years |
| $T_{1/2}$ | Radioactive half-life | Years |

The $SSL_{T_{1/2}}$ equation for an organic analyte which includes first-order degradation is:

$$SSL_{T_{1/2}} = \frac{MCL \cdot DAF \cdot \left(K_d + \frac{\theta_w + H \cdot \theta_a}{\rho_\beta} \right)}{e^{(-0.693 \cdot T_{MEAN} / T_{1/2})}} / [1000 \text{ ug/mg}] \quad (8d)$$

Where:

Table 4-11. Parameters for $SSL_{T_{1/2}}$ Equation for Organics

| Parameter | Definition | Units |
|-----------------|---|----------|
| $SSL_{T_{1/2}}$ | Degradation Adjusted Soil Screening Level | mg/kg |
| MCL | Maximum Contaminant Level, PRG | mg/L |
| DAF | Dilution Attenuation Factor | Unitless |
| K_d | Distribution coefficient | L/kg |
| ρ_β | Soil bulk density | Kg/L |
| θ_w | Volumetric moisture content | Percent |
| T_{Mean} | Mean travel time to top of aquifer | Years |
| $T_{1/2}$ | Degradation half-life | Years |

Finally, the groundwater equilibrium equations are arranged to be the reciprocal of the $SSL_{T_{1/2}}$ equations. The $SSL_{T_{1/2}}$ may be substituted for the input soil concentration, and the resulting groundwater concentration will exactly equal the MCL or PRG. This same relationship is true for any of the analytical classes and provides a simple checking procedure for these calculations, i.e., substitute $SSL_{T_{1/2}}$ for C_t on the input sheet, then $C_{gw} = MCL$.

The following equation is used to calculate the default SSL for all organic analytes and mercury:

$$SSL = MCL \cdot DAF \cdot \left(K_d + \frac{\theta_w + H \cdot \theta_a}{\rho_\beta} \right) / [1000 \text{ ug/mg}] \quad (8e)$$

The following equation is used to calculate the default SSL for inorganic analytes:

$$SSL = MCL \cdot DAF \cdot \left(K_d + \frac{\theta_w}{\rho_\beta} \right) / [1000 \text{ ug/mg}] \quad (8f)$$

The following equation is used to calculate the default SSL for radiological analytes:

$$SSL = MCL \cdot DAF \cdot [0.001 \text{ kg/g}] \cdot \left(K_d + \frac{\theta_w}{\rho_\beta} \right) \quad (8g)$$

4.8 Calculation of the MLSSL

All MLSSL values are based on the same basic equation. The equation shown below is used for all classes of analytes except radionuclides:

$$MLSSL = \frac{(MCL \cdot DAF \cdot I \cdot ED)}{(\rho_{\beta} \cdot d_s)} / [1000 \text{ ug/mg}] \quad (9a)$$

Where:

Table 4-12. Parameters for MLSSL Equation for Organics, Inorganics and Metals

| Parameter | Definition | Units |
|----------------|---|----------|
| MLSSL | Mass Limited Soil Screening Level | mg/kg |
| MCL | Maximum Contaminant Level, PRG | ug/L |
| DAF | Dilution Attenuation Factor | Unitless |
| I | Infiltration Rate through the vadose zone | Ft/yr |
| ED | Exposure Duration (70 years) | Years |
| ρ_{β} | Soil Bulk Density | Kg/L |
| d_s | Vertical thickness of source | Feet |

The MLSSL equation for a radionuclide uses equation 9a with a conversion factor and decay term, as follows:

$$MLSSL_{T_{1/2}} = \frac{(MCL \cdot DAF \cdot I \cdot ED \cdot [0.001 \text{ kg/g}])}{(\rho_{\beta} \cdot d_s)} \times \frac{1}{e^{(-0.693 \cdot ED / T_{1/2})}} \quad (9b)$$

Where:

Table 4-13. Parameters for Decay Adjusted MLSSL Equation for Radionuclides

| Parameter | Definition | Units |
|-------------------|--|----------|
| $MLSSL_{T_{1/2}}$ | Decay adjusted Mass Limited Soil Screening Level | pCi/g |
| MCL | Maximum Contaminant Level, PRG | pCi/L |
| DAF | Dilution Attenuation Factor | Unitless |
| I | Vertical infiltration Rate through the vadose zone | Ft/yr |
| ED | Exposure Duration (70 years) | Years |
| ρ_{β} | Soil Bulk Density | Kg/L |
| d_s | Vertical thickness of source | Feet |
| $T_{1/2}$ | Radioactive decay half-life | Years |

Soil Saturation Limit in Soils for Organic Compounds

The C_{sat} is the contaminant concentration in soil at which the absorptive limits of the soil particles, the solubility limits in the pore water, and the saturation of soil-pore air have been reached. Above this concentration, the soil contaminant may be present in free phase, i.e., NAPLs for contaminants that are liquid at ambient soil temperatures and pure solid phases for compounds that are solid at ambient soil temperatures. The C_{sat} equation is an equilibrium equation that partitions vapor, sorbed, and liquid phases from an upper bound limit, which is the aqueous solubility limit of the compound. A NAPL can exist above the C_{sat} threshold.

Users should exercise caution when they interpret C_{sat} data in the model. C_{sat} limits apply to pure phase contaminants, not to mixtures of organic compounds. For mixtures, the C_{sat} level for any individual component will be lower than the pure phase C_{sat} limit. If mixtures occur, a different calculation method is required to account for the physical changes of the mixture, i.e., lower solubility, vapor pressure, etc. Therefore, any exceedence of a C_{sat} threshold should be regarded as a serious potential for the presence of NAPL in soil, and a detailed assessment of the data should be performed.

The addition of C_{sat} screening in the model is an enhancement from earlier versions.

The following SSL equation is needed to calculate the C_{sat} threshold in soil:

$$C_{sat} = \frac{S}{\rho_{\beta}} \cdot (K_d \cdot \rho_{\beta} + \theta_w + H \cdot \theta_a) \quad (10)$$

where:

S is the aqueous solubility limit of an organic compound.

Screening Tests

The result modules contain multiple screening criteria to automatically interpret the numerical data computed by the model. The screening criteria are called arguments and are in the form of logic functions embedded in the model code. These logic functions are very important to understand because they provide the technical basis for the decisions that the software generates. The logic functions are based upon criteria from the FFA Contaminant Migration Protocol and Soil Screening Guidance. Three logic arguments are associated with the result module:

1. Is the groundwater concentration “greater than or equal to” the MCL? In partial code form: $C_{gw} \geq MCL$.
2. Is the mean travel time less than or equal to the evaluation time (formerly 1,000 years)? In partial code form: $T_{Mean} \leq T_e$.
3. Is the waste unit soil concentration greater than or equal to the MLSSL? In partial code form: $C_t \geq MLSSL$.

Therefore, the partial code form of the compound logic argument would look like this:

Logic Screening Argument String

$$IF(AND(C_{gw} \geq MCL, T_{Mean} \leq T_e, C_t \geq MLSSL), \text{value if true, value if false}) \quad (11)$$

Table 4-14. Summary of Screening Decision Logic

| • Argument | • Decision Logic Argument Matrix | | | | | | | |
|-------------------------------|----------------------------------|-------------|-------|-------|-------|-------|-------|-------|
| • $C_{gw} \geq MCL$ | True | True | True | True | False | False | False | False |
| • $T_{Mean} \leq T_e$ | True | True | False | False | False | False | True | True |
| • $C_t \geq MLSSL$ | False | True | True | False | True | False | False | True |
| • Screening Logic Test Result | Pass | Fail | Pass | Pass | Pass | Pass | Pass | Pass |

Note: All logic tests are connected by <and> operator.

The table presents the possible 24 permutations for the logical tests. This means all three logic tests must evaluate to “TRUE” in order to “FAIL” the screening logic test. As illustrated in the Table 4-8, there is only one set of logical values that can produce a failed screening comparison.

Because of the relative confusion caused by the terms “True”, “False”, “Fail”, “Pass”, the name of the analyte is automatically listed by model in the appropriate column as having failed the screening criteria. “FAIL” in the context of the software, means that this analyte is a contaminant migration constituent of concern (CMCOC) and should be retained for further analysis.

Operational Order

Generally, the spreadsheet model operates according to the following steps:

1. Input the unit-specific hydrogeologic or default data into the Mixing Zone and Dilution Attenuation Factor Calculation spreadsheet #1.
2. Enter geotechnical unit-specific and hydrogeologic data into spreadsheets #2 and #3.
3. Enter total soil mass concentrations (C_i) into the appropriate chemical-specific input spreadsheets 4A through 4E. The chemical-specific input spreadsheets are organized by analytical fraction, i.e., volatile organic compounds (VOCs), semi-volatile organic compounds (SVOCs), pesticides/PCBs (Pest/PCBs), metals (Metals) and radionuclides (RADs).
4. Observe or print the results from the Result spreadsheets 5A through 5E. The result spreadsheets are also organized by analytical fraction.

5. Chemical-specific values may be adjusted by “Unprotecting” the input spreadsheets and changing the K_{oc} , f_{oc} , Henry’s Law Constant, half-life variable or solubility.
6. Use the “Format SSL” command button on the result spreadsheets to automatically perform an SSL and C_{sat} soil screening.

The result spreadsheets will auto-calculate and list the analytes that have mean travel times less than the evaluation time and exceed their respective MCL, risk-based concentration (PRG), or risk-based activity (RBA). The mean travel time, groundwater concentration, $SSL_{T1/2}$ -RGO, $MLSSL$ -RGO, and SSL -RGO will be calculated for each analyte for which a soil concentration (C_i) has been entered.

5.0 RESULTS

The desired output from the computer code is specified in the table below. A copy of the computer output is provided in Attachment 1.

Table 5-1. Output From VZCOMML, V3 for E-7 Test Run

| Calculated Parameter | Calculated Result | Units |
|--|-------------------|---------------|
| Mixing Zone Depth | 11.94 | Feet |
| DAF | 3.08 | Dimensionless |
| Pore-water Velocity | 5.929 | Feet/year |
| K _d for Trichloroethylene (TCE) | 0.795 | Liters/kg |
| Retardation (TCE) | 7.4 | Unitless |
| Mean Travel Time (TCE) | 99.99 | Years |
| Groundwater Concentration (TCE) | 1.56 | µg/L |
| SSL _{T1/2} – RGO (TCE) | 16.1 | mg/kg |
| MLSSL – RGO (TCE) | 0.113 | mg/kg |
| Default SSL-RGO (TCE) | .0156 | mg/kg |
| Retardation for Technetium-99 | 1.8 | Unitless |
| Mean Travel Time (Tc-99) | 24.37 | Years |
| Groundwater Concentration (Tc-99) | 1,040.0 | pCi/L |
| SSL _{T1/2} – RGO (Tc-99) | 0.867 | pCi/g |
| MLSSL – RGO (Tc-99) | 20.4 | pCi/g |
| Default SSL – RGO (Tc-99) | 0.867 | pCi/g |
| C _{sat} (TCE) | 1120.0 | mg/kg |

It should be noted that the logic tests contained within the VOC result module should not be highlighted. “Trichloroethylene” will not be flagged as failing the screening. Conversely, on the RAD results module, even though the calculated groundwater concentration of 1,040.0 pCi/L exceeds the MCL of 900 pCi/L, Tc-99 is not highlighted in red because of the mass balance logic argument. The mass balance logic argument checks the MLSSL and compares it to the input soil concentration. If the MLSSL value is greater than the input soil concentration, the analyte is not flagged even though the groundwater concentration exceeds the MCL. This indicates the logic arguments are returning the appropriate values according to the matrix in Table 4-13.

6.0 CONCLUSIONS

Table 5-1 illustrates the model result output. The model calculates important contaminant transport parameters for any analyte on the TAL/TCL list plus a radionuclide suite. The parameters of greatest relevance will probably be the mean travel time, the groundwater concentration, SSL_{T1/2}, and MLSSL. The model is flexible in that it can incorporate a high degree of unit-specific, SRS-specific, USEPA default, and

chemical-specific variables. Hydrogeologic, geotechnical, and chemical-specific inputs should be adjusted to match the CSM to represent actual conditions at the waste unit. Additionally, the model is consistent with the USEPA guidance in that it utilizes similar approaches and parameters, equations and reciprocal equations as outlined in USEPA's soil screening guidance (USEPA 1996). According to USEPA nomenclature, the model would be classified as a "detailed site-specific model." The model allows for hypothetical scenarios as well as "what-if" scenarios. The model is easy to use in that it requires a minimum of simple, easily measured data. The updated version accounts for fundamental fate and transport processes in the solid, aqueous, and vapor phases with equilibrium partitioning equations.

By design, the model incorporates intentionally conservative assumptions, including the calculation of SSLs. The assumption that the source of the analyte is infinite and uniformly distributed to the depth of detection at an average concentration is conservative and overestimates the mass of an analyte where analytes are only sporadically detected. Alternatively, localized hot spots may not be adequately addressed by averaging although analyte concentrations in soils impacted by liquid effluent discharges should be relatively homogeneous. The receptor well is conservatively placed adjacent to the waste unit; therefore, the dilution that would occur when clean water is withdrawn from the receptor well is not included. This effect becomes more important when the source of the release is of small areal extent such as a pipeline leak, i.e., limited mass. The vadose fate and transport model assumes that the entire mass of an analyte is mobile when, for many metals and radionuclides, a large fraction is immobile (complexed in the soils). The K_{ds} that are utilized are predominantly for sand, when in reality the geology is a heterogeneous system of sand, silt clay, and organic matter. This heterogeneous stratigraphy also impacts results in variable vertical hydraulic conductivity, which may significantly slow infiltration through the vadose zone but was not accounted for in this calculation.

Version 3 includes a number of enhancements, including the vadose zone form of the retardation coefficient equation. By incorporating the moisture content into the retardation coefficient equation, it mimics the behavior of water flow in unsaturated soils to coincide with the observed behavior of hydraulic conductivity and pore-water velocity. The new version also screens total contaminant concentrations against soil saturation limits. This is an important feature in determining if NAPL may be present in any of the samples collected at a waste unit.

The previous version used a truncated form of equilibrium partitioning equation that did not distribute mass to vapor or liquid phases. The new version incorporates complete equilibrium partitioning equations to account for the distribution of mass in solid, liquid and vapor phases. This change makes the model significantly more complicated. Whereas the previous versions used one type of equilibrium equation, the new version uses twelve or more different equations to account for the distribution of mass by different chemical classes. Users should be aware that the results generated with Version 3.0 will not be numerically comparable to the output from previous versions.

Additional enhancements in Version 3 included changing the evaluation time (T_e) to a user-defined variable. This enhancement makes the software more flexible in considering alternative times based upon site-specific conditions or a variety of exposure alternatives. The software also included an upgrade to expand the output data display for vadose zone characteristics.

The model also calculates a variety of possible SSLs/RGOs to assist in remedial decisions at a waste unit and to evaluate the effectiveness of various remedial action alternatives.

7.0 REFERENCES

Denham, M.E. 1996, *Appropriate Kd Values for SCDF Project Including C-14 and Np-237*, SRT-ESS-96-350, Savannah River Site, Aiken, SC., personal memorandum to P. M. Garrett dated July 23, 1996

Electronic Handbook of Risk Assessment Values, Volume 6, Issue 1/2, (c), Electronic Handbook Publishers, Inc., February 1997

Flach, G. P. et al., 1996, *Groundwater Flow and Tritium Migration from the SRS Old Burial Ground to Fourmile Branch (U)*, Savannah River Site, Aiken, SC., WSRC-TR-0106

Freeze, R. A., J. A. Cherry, 1979. *Groundwater*, Prentice-Hall Inc, Englewood, Cliffs, N.J.

Hoeffner, S.L., 1985, *Radionuclide Sorption on Savannah River Plant Burial Ground Soil - A Summary and Interpretation of Laboratory Data*, DP-1702, E.I. du Pont de Nemours & Company, Savannah River Laboratory, Aiken, SC

Hornberger, G. M., R. B. Clapp, 1978. "Empirical Equations for Some Soil Hydraulic Properties," *Water Resources Journal*, Vol. 14, No. 4, pp 601-604, August

Howard, P.H. et al., 1991. *Handbook of Environmental Degradation Rates*, Lewis Publishers

Looney, B.B., Grant, M.W., and King, C.M., 1987. *Estimation of Geochemical Parameters for Assessing Subsurface Transport at the Savannah River Plant*, DPST-85-903, Savannah River Plant, Aiken, SC

Rucker, Gregory G., 1996. Soil Screening Calculator, Copyright SRS-96-507C, Savannah River Site, Aiken, SC.

Rucker, Gregory G. 1998. Vadose Zone Contaminant Migration Model, Copyright SRS-98-530C, Savannah River Site, Aiken, SC.

Rucker, Gregory G. 1999. Multi-Layer Contaminant Migration Model (VZCOMML), Copyright SRS-99-513C, License #LA-01-002, Savannah River Site, Aiken, SC.

Rucker, Gregory G. 1999. Vadose Zone Contaminant Fate and Transport Model, K-CLC-G-00051, Savannah River Site, Aiken, SC.

Rucker, Gregory G. 1999. Multi-Layered Calculation of Pore-Water Velocity in the Vadose Zone, Q-CLC-B-00002, Savannah River Site, Aiken, SC.

Safe Drinking Water Act, 40 CFR 141.16

Sheppard, M.I., Thibault, D.H., 1990, "Default Soil Solid/Liquid Partition Coefficients, K_{ds} for Four Major Soil Types: A Compendium," *Health Physics*, 59(4), 471-482

USEPA, National Interim Primary Drinking Water Regulations, EPA-570/9-76-003

USEPA, 1988. Superfund Exposure Assessment Manual, EPA/540/1-88/001.

USEPA, 1996, *Technical Background Document for Soil Screening Guidance*, EPA 540/R-95/128, August

USEPA, 2000. *Soil Screening Guidance for Radionuclides: Technical Background Guidance Document*, EPA/540-R-00-006, October

8.0 ATTACHMENTS

Attachment 1 Example Output for VZCOMML E-7 Test Run

ATTACHMENT 1

Example Output for VZCOMML E-7 Test Run

| ESTIMATION OF MIXING ZONE DEPTH | | | |
|---|---------|-----------|--|
| PROJECT NAME: | | | |
| Calculation of Mixing Zone ¹ | | | |
| Variable | Default | Units | Parameter |
| | 0.0112 | | Constant |
| L= | 60 | feet | Source length parallel to groundwater flow |
| I= | 1.25 | feet/year | Infiltration rate |
| K= | 1449 | feet/year | Aquifer hydraulic conductivity |
| da= | 100 | feet | Aquifer thickness |
| g= | 0.009 | feet/feet | Hydraulic gradient |
| | | | |
| d= | 11.94 | feet | Mixing Zone Depth |
| | | | |
| DILUTION ATTENUATION FACTOR | | | |
| Calculation of DAF ² | | | |
| | | | |
| Variable | Default | Units | Parameter |
| K= | 1449 | feet/year | Aquifer hydraulic conductivity |
| g= | 0.009 | feet/feet | Hydraulic gradient |
| mz= | 11.94 | feet | Mixing Zone Depth |
| I= | 1.25 | feet/year | Infiltration rate |
| L= | 60 | feet | Source length parallel to groundwater flow |
| | | | |
| DAF= | 3.08 | | 3/22/2004 8:11 |

| Parameter | Variable | Value | Units |
|---------------------------------------|-----------------|---------|--------------------|
| Depth of Contamination Beneath Source | d _s | 7.00 | feet |
| Exposure Duration | ED | 70.00 | years |
| Approximate Depth to Groundwater | L _v | 80.00 | feet |
| Evaluation Time | T _e | 1000.00 | years |
| Bulk Density | P _b | 1.70 | kilograms/liter |
| Fraction Organic Carbon | f _{oc} | 0.0030 | fraction (decimal) |

| CALCULATION OF PORE-WATER VELOCITY | | MOISTURE CONTENT AND POROSITY DATA SUMMARY FOR SOURCE LAYER | | | | |
|---|-----------------|---|--------------------------------------|--|---|---|
| Source Layer | Enter Values | Vertical Thickness Th (feet) | Moisture Content θ (fraction) | Effective Moisture Content θ_e (fraction) | Water-Filled Porosity θ_w (fraction) | Air-Filled Porosity θ_a (fraction) |
| Saturated Effective Porosity | 7 | 7.00 | 0.3624 | 0.2718 | 0.3624 | 0.0376 |
| Select Soil Texture | Silly Clay | | | | | |
| "K" Parameter | 16 | | | | | |
| "b" Parameter | 11.4 | | | | | |
| Layer 1 (beneath source) | | | | | | |
| Thickness | 10 | | | | | |
| Total Porosity | 0.40 | | | | | |
| Saturated Effective Porosity | 0.30 | | | | | |
| Select Soil Texture | Sandy Clay Loam | | | | | |
| "K" Parameter | 131 | | | | | |
| "b" Parameter | 7.12 | | | | | |
| Layer 2 (beneath source) | | | | | | |
| Thickness | 50 | | | | | |
| Total Porosity | 0.40 | | | | | |
| Saturated Effective Porosity | 0.25 | | | | | |
| Select Soil Texture | Silly Clay | | | | | |
| "K" Parameter | 16 | | | | | |
| "b" Parameter | 11.4 | | | | | |
| Layer 3 (beneath source) | | | | | | |
| Thickness | 10 | | | | | |
| Total Porosity | 0.40 | | | | | |
| Saturated Effective Porosity | 0.22 | | | | | |
| Select Soil Texture | Sand | | | | | |
| "K" Parameter | 1772 | | | | | |
| "b" Parameter | 4.38 | | | | | |
| Layer 4 (beneath source) | | | | | | |
| Thickness | 10 | | | | | |
| Total Porosity | 0.44 | | | | | |
| Saturated Effective Porosity | 0.25 | | | | | |
| Select Soil Texture | Sandy Clay Loam | | | | | |
| "K" Parameter | 43 | | | | | |
| "b" Parameter | 7.75 | | | | | |
| Weighted Average | | | | | | |
| Sum of Layers 1 - 4 | 80.00 | | 0.3371 | 0.2708 | 0.4050 | 0.2525 |
| Sum of Layers 1 - 4 | | | | | | |
| Pore-Water Velocity (Vs) Layers 1 - 4 (feet/year) | 5.9290 | | | | | |
| | 8/6/2004 12:28 | | | | | |

| Soil Texture | "K" Parameter Estimates Ks (ft/y) | Soil-Specific Exponential Parameter, b |
|-----------------|-----------------------------------|--|
| Sand | 6004 | 4.05 |
| Loamy Sand | 1772 | 4.38 |
| Sandy Loam | 755 | 4.9 |
| Silly Loam | 394 | 5.3 |
| Loam | 197 | 5.39 |
| Sandy Clay Loam | 131 | 7.12 |
| Silly Clay Loam | 43 | 7.75 |
| Clay Loam | 66 | 8.52 |
| Sandy Clay | 33 | 10.4 |
| Silly Clay | 26 | 10.4 |
| Clay | 16 | 11.4 |

Source: EPA, 1986. Technical Background Document for Soil Screening Guidance. EPA 540/R-95/128. August 1986.

| Volatile Organic Analytes | Koc (VOC) L/Kg | Kd ¹⁰ (VOC) L/Kg | T1/2 (VOC) Years | H' (VOC) Dimensionless | S (VOC) mg/L | C _t (VOC) mg/kg |
|---|----------------------|-----------------------------------|------------------------|------------------------------|--------------------|----------------------------------|
| 1,1,1-Trichloroethane | 1.35E+02 | 4.05E-01 | 7.50E-01 | 7.05E-01 | 1.33E+03 | |
| 1,1,2,2-Tetrachloroethane | 7.90E+01 | 2.37E-01 | 1.23E-01 | 1.41E-02 | 2.97E+03 | |
| 1,1,2-Trichloroethane | 7.50E+01 | 2.25E-01 | 1.00E+00 | 3.74E-02 | 4.42E+03 | |
| 1,1-Dichloroethane | 5.34E+01 | 1.60E-01 | 4.23E-01 | 2.30E-01 | 5.06E+03 | |
| 1,1-Dichloroethylene | 6.50E+01 | 1.95E-01 | 5.00E-01 | 1.07E+00 | 2.25E+03 | |
| 1,2-Dichloroethane | 3.80E+01 | 1.14E-01 | 5.00E-01 | 4.01E-02 | 8.52E+03 | |
| 1,2-Dichloroethylene | 6.50E+01 | 1.85E-01 | 5.00E-01 | 2.71E-01 | 6.30E+03 | |
| 1,2-Dichloropropane | 4.70E+01 | 1.41E-01 | 3.50E+00 | 1.15E-01 | 2.80E+03 | |
| 2-Hexanone | 1.94E+01 | 5.82E-02 | 3.80E-02 | 1.54E-03 | 3.50E+04 | |
| Acetone | 2.20E+00 | 6.60E-03 | 1.90E-02 | 1.59E-03 | 1.00E+06 | |
| Benzene | 6.17E+01 | 1.85E-01 | 4.40E-02 | 2.28E-01 | 1.75E+03 | |
| Bromodichloromethane | 5.50E+01 | 1.65E-01 | 5.00E-02 | 6.56E-02 | 6.74E+03 | |
| Bromoform | 1.26E+02 | 3.78E-01 | 5.00E-01 | 2.19E-02 | 3.10E+03 | |
| Bromomethane (Methyl bromide) | 9.00E+00 | 2.70E-02 | 7.70E-02 | 2.56E-01 | 1.52E+04 | |
| Carbon disulfide | 5.40E+01 | 1.62E-01 | 9.34E-03 | 1.24E+00 | 1.19E+03 | |
| Carbon tetrachloride | 1.52E+02 | 4.56E-01 | 1.00E+00 | 1.25E+00 | 7.93E+02 | |
| Chlorobenzene | 2.24E+02 | 6.72E-01 | 4.11E-01 | 1.52E-01 | 4.72E+02 | |
| Chloroethane | 1.50E+01 | 4.50E-02 | 7.70E-02 | 8.20E-02 | 5.74E+03 | |
| Chloroethene (Vinyl chloride) | 8.20E+00 | 2.46E-02 | 5.00E-01 | 1.11E+00 | 2.76E+03 | |
| Chloroform | 5.25E+01 | 1.58E-01 | 5.00E-01 | 1.50E-01 | 7.92E+03 | |
| Chloromethane (Methyl chloride) | 5.50E+00 | 1.65E-02 | 7.70E-02 | 4.06E-01 | 6.50E+03 | |
| cis-1,3-Dichloropropene | 2.71E+01 | 8.13E-02 | 3.10E-02 | 7.26E-01 | 2.80E+03 | |
| Dibromochloromethane | 1.07E+02 | 3.21E-01 | 5.00E-01 | 1.88E-01 | 4.54E+03 | |
| Dichloromethane (Methylene chloride) | 1.00E+01 | 3.00E-02 | 3.07E-01 | 8.98E-02 | 1.30E+04 | |
| Ethylbenzene | 2.04E+02 | 6.12E-01 | 2.70E-02 | 3.23E-01 | 1.69E+02 | |
| Methyl ethyl ketone | 4.51E+00 | 1.35E-02 | 1.90E-02 | 2.10E-03 | 2.68E+05 | |
| Methyl isobutyl ketone (4-Methyl-2-pentanone) | 1.90E+01 | 5.70E-02 | 1.90E-02 | 2.78E-03 | 1.90E+04 | |
| Styrene | 9.12E+02 | 2.74E+00 | 7.70E-02 | 1.13E-01 | 3.10E+02 | |
| Tetrachloroethylene | 2.65E+02 | 7.95E-01 | 1.00E+01 | 7.54E-01 | 2.00E+02 | |
| Toluene | 1.40E+02 | 4.20E-01 | 6.00E-02 | 2.72E-01 | 5.26E+02 | |
| trans-1,3-Dichloropropene | 4.80E+01 | 1.44E-01 | 3.10E-02 | 5.33E-02 | 2.80E+03 | |
| Trichloroethylene | 2.65E+02 | 7.95E-01 | 1.00E+01 | 4.22E-01 | 1.10E+03 | 5.00E+00 |
| Vinyl acetate | 1.70E+01 | 5.10E-02 | 3.97E-02 | 2.10E-02 | 2.00E+04 | |
| Xylenes | 2.38E+02 | 7.14E-01 | 7.70E-02 | 2.13E-01 | 1.61E+02 | |

| Radiological Analytes | Koc (RAD) L/Kg | Kd ¹⁰ (RAD) L/kg | T1/2 (RAD) Years | C _t (RAD) pCi/g |
|-----------------------|----------------------|-----------------------------------|------------------------|----------------------------------|
| Actinium-228 | NA | 4.50E+02 | 7.00E-04 | |
| Americium-241 | NA | 1.00E+02 | 4.32E+02 | |
| Americium-243 | NA | 1.00E+02 | 7.38E+03 | |
| Antimony-124 | NA | 4.00E+03 | 1.65E-01 | |
| Antimony-125 | NA | 4.00E+03 | 2.77E+00 | |
| Carbon-14 | NA | 2.00E+01 | 5.73E+03 | |
| Cesium-134 | NA | 5.00E+02 | 2.06E+00 | |
| Cesium-137 | NA | 5.00E+02 | 3.02E+01 | |
| Cobalt-57 | NA | 1.00E+01 | 7.42E-01 | |
| Cobalt-60 | NA | 1.00E+01 | 5.27E+00 | |
| Curium-242 | NA | 3.10E+03 | 4.47E-01 | |
| Curium-243/244 | NA | 3.10E+03 | 2.85E+01 | |
| Curium-245/246 | NA | 3.10E+03 | 8.50E+03 | |
| Curium-247 | NA | 3.10E+03 | 1.56E+07 | |
| Europium-152 | NA | 2.45E+02 | 1.36E+01 | |
| Europium-154 | NA | 2.45E+02 | 8.80E+00 | |
| Europium-155 | NA | 2.45E+02 | 4.96E+00 | |
| Iodine-129 | NA | 3.60E+00 | 1.57E+07 | |
| Lead-212 | NA | 2.70E+02 | 1.20E-03 | |
| Manganese-54 | NA | 5.00E+01 | 8.58E-01 | |
| Neptunium-237 | NA | 1.00E+01 | 2.14E+06 | |
| Neptunium-239 | NA | 1.00E+01 | 6.50E-03 | |
| Nickel-63 | NA | 6.50E+01 | 1.00E+02 | |
| Plutonium-238 | NA | 1.00E+02 | 8.78E+01 | |
| Plutonium-239/240 | NA | 1.00E+02 | 2.41E+04 | |
| Potassium-40 | NA | 7.50E+01 | 1.28E+09 | |
| Promethium-147 | NA | 2.40E+02 | 2.62E+00 | |
| Radium-226 | NA | 1.00E+02 | 1.60E+03 | |
| Radium-228 | NA | 1.00E+02 | 5.75E+00 | |
| Sodium-22 | NA | 1.00E+02 | 2.60E+00 | |
| Strontium-90 | NA | 8.00E+00 | 2.86E+01 | |
| Technetium-99 | NA | 1.00E-01 | 2.17E+05 | 1.00E+00 |
| Thorium-228 | NA | 1.00E+02 | 1.91E+00 | |
| Thorium-230 | NA | 1.00E+02 | 7.70E+04 | |
| Thorium-232 | NA | 1.00E+02 | 1.41E+10 | |
| Uranium-233/234 | NA | 4.00E+01 | 2.45E+05 | |
| Uranium-235 | NA | 4.00E+01 | 7.04E+08 | |
| Uranium-238 | NA | 4.00E+01 | 4.47E+09 | |
| Zinc-65 | NA | 6.20E+01 | 6.68E-01 | |
| Zirconium-95 | NA | 6.00E+02 | 1.75E-01 | |

Engineering Calculation
 Modifications of the Vadose Zone Contaminant Migration Multi-Layer Model
 April 1, 2004

K-CLC-G-00051
 Revision 0
 Sheet 42 of 44

| Volatile Organic Analytes | Retardation ⁴ R (VOC) (Unitless) | Mean Travel Time ⁵ Tt (VOC) (years) | Groundwater ⁶ Concentration Cw (VOC) in Aquifer (ug/L) | MCL or PRG Action Level (ug/L) | Analytes Greater Than MCL/PRG/MLSSL and Less Than Evaluation Time (T _e) | SSL-T1/2 ⁷ T1/2-SSL RGO (mg/kg) | MLSSL ⁸ SSL-ML RGO (mg/kg) | Default ⁹ SSL RGO (mg/kg) |
|---|---|---|--|--------------------------------------|--|--|---|--|
| 1,1,1-Trichloroethane | 4.3 | 57.56 | 0.00E+00 | 200 | | 4.87E+22 | 4.52E+00 | 3.90E-01 |
| 1,1,2,2-Tetrachloroethane | 2.9 | 39.28 | 0.00E+00 | 0.055 | | 9.81E+91 | 1.24E-03 | 7.62E-05 |
| 1,1,2-Trichloroethane | 2.8 | 37.97 | 0.00E+00 | 5.0 | | 1.81E+09 | 1.13E-01 | 6.75E-03 |
| 1,1-Dichloroethane | 2.3 | 30.92 | 0.00E+00 | 810 | | 9.46E+21 | 1.83E+01 | 9.43E-01 |
| 1,1-Dichloroethylene | 2.6 | 34.71 | 0.00E+00 | 7.0 | | 7.26E+18 | 1.58E-01 | 9.30E-03 |
| 1,2-Dichloroethane | 1.9 | 25.90 | 0.00E+00 | 5.0 | | 1.95E+13 | 1.13E-01 | 5.05E-03 |
| 1,2-Dichloroethylene | 2.6 | 34.71 | 0.00E+00 | 70 | | 6.96E+19 | 1.58E+00 | 8.92E-02 |
| 1,2-Dichloropropane | 2.1 | 28.83 | 0.00E+00 | 5.0 | | 1.65E+00 | 1.13E-01 | 5.49E-03 |
| 2-Hexanone | 1.5 | 19.83 | 0.00E+00 | NA | | PARAMETER | PARAMETER | PARAMETER |
| Acetone | 1.1 | 14.21 | 0.00E+00 | 610 | | 5.27E+224 | 1.38E+01 | 4.12E-01 |
| Benzene | 2.5 | 33.63 | 0.00E+00 | 5.0 | | 6.90E+227 | 1.13E-01 | 6.20E-03 |
| Bromodichloromethane | 2.3 | 31.44 | 0.00E+00 | 0.18 | | 3.98E+185 | 4.07E-03 | 2.10E-04 |
| Bromoform | 4.0 | 54.62 | 0.00E+00 | 10 | | 1.37E+31 | 2.26E-01 | 1.82E-02 |
| Bromomethane (Methyl bromide) | 1.2 | 16.43 | 0.00E+00 | 8.7 | | 1.09E+62 | 1.97E-01 | 6.58E-03 |
| Carbon disulfide | 2.3 | 31.12 | 0.00E+00 | 1000 | | PARAMETER | 2.26E+01 | 1.24E+00 |
| Carbon tetrachloride | 4.7 | 63.11 | 0.00E+00 | 5.0 | | 1.05E+17 | 1.13E-01 | 1.07E-02 |
| Chlorobenzene | 6.4 | 86.61 | 0.00E+00 | 100 | | 7.19E+62 | 2.26E+00 | 2.73E-01 |
| Chloroethane | 1.4 | 18.39 | 0.00E+00 | 4.6 | | 2.76E+69 | 1.04E-01 | 3.68E-03 |
| Chloroethene (Vinyl chloride) | 1.2 | 16.17 | 0.00E+00 | 2.0 | | 8.72E+06 | 4.52E-02 | 1.61E-03 |
| Chloroform | 2.3 | 30.63 | 0.00E+00 | 80 | | 2.51E+17 | 1.81E+00 | 9.20E-02 |
| Chloromethane (Methyl chloride) | 1.1 | 15.29 | 0.00E+00 | 1.5 | | 6.28E+56 | 3.39E-02 | 1.10E-03 |
| cis-1,3-Dichloropropene | 1.7 | 22.34 | 0.00E+00 | 0.4 | | 2.86E+213 | 9.05E-03 | 3.82E-04 |
| Dibromochloromethane | 3.6 | 48.42 | 0.00E+00 | 80 | | 1.85E+28 | 1.81E+00 | 1.32E-01 |
| Dichloromethane (Methylene chloride) | 1.2 | 16.76 | 0.00E+00 | 5 | | 1.03E+14 | 1.13E-01 | 3.77E-03 |
| Ethylbenzene | 5.9 | 80.08 | 0.00E+00 | 700 | | PARAMETER | 1.58E+01 | 1.79E+00 |
| Methyl ethyl ketone | 1.1 | 14.96 | 0.00E+00 | 1900 | | 1.49E+237 | 4.30E+01 | 1.33E+00 |
| Methyl isobutyl ketone | 1.5 | 19.69 | 0.00E+00 | 160 | | PARAMETER | 3.62E+00 | 1.33E-01 |
| Styrene | 23.1 | 311.17 | 0.00E+00 | 100 | | PARAMETER | 2.26E+00 | 9.08E-01 |
| Tetrachloroethylene | 7.4 | 99.99 | 0.00E+00 | 5.0 | | 1.61E+01 | 1.13E-01 | 1.58E-02 |
| Toluene | 4.4 | 59.19 | 0.00E+00 | 1000 | | 1.55E+297 | 2.26E+01 | 1.97E+00 |
| trans-1,3-Dichloropropene | 2.2 | 29.16 | 0.00E+00 | 0.4 | | 5.59E+279 | 9.05E-03 | 4.41E-04 |
| Trichloroethylene | 7.4 | 99.99 | 1.56E+00 | 5.0 | | 1.60E+01 | 1.13E-01 | 1.56E-02 |
| Vinyl acetate | 1.4 | 19.04 | 0.00E+00 | 410 | | 7.57E+143 | 9.27E+00 | 3.34E-01 |
| Xylenes | 6.8 | 91.18 | 0.00E+00 | 10000 | | PARAMETER | 2.26E+02 | 2.87E+01 |
| 8/6/2004 12:39 | | | | | | | | |
| PARAMETER indicates that a variable within the equation is not available such as the Kd or T1/2 or the source concentration has been decayed to zero. | | | | | | | | |

Engineering Calculation
Modifications of the Vadose Zone Contaminant Migration Multi-Layer Model
April 1, 2004

K-CLC-G-00051
Revision 0
Sheet 43 of 44

| Radiological Analytes | Retardation ⁴ R (RAD) (Unitless) | Mean Travel Time Tt (RAD) (years) | Groundwater ⁶ Concentration Cw (RAD) in Aquifer (pCi/L) | MCL Action Level (RAD) (pCi/L) | Analytes Greater Than MCL/PRG/MLSSL and Less Than Evaluation Time (T _e) | SSL-T1/2 ⁷ T1/2-SSL RGO (pCi/g) | MLSSL-T1/2 ⁸ SSL-ML RGO (pCi/g) | Default ⁹ SSL RGO (pCi/g) |
|-----------------------|---|--|---|--------------------------------------|--|--|--|--|
| Actinium-228 | 3629.6 | 48973.49 | 0.00E+00 | 15 | | PARAMETER | PARAMETER | 2.08E+01 |
| Americium-241 | 807.3 | 10893.49 | 0.00E+00 | 15 | | 1.80E+08 | 3.80E-01 | 4.62E+00 |
| Americium-243 | 807.3 | 10893.49 | 0.00E+00 | 15 | | 1.29E+01 | 3.41E-01 | 4.62E+00 |
| Antimony-124 | 32255.0 | 435213.49 | 0.00E+00 | 60 | | PARAMETER | 6.53E+127 | 7.38E+02 |
| Antimony-125 | 32255.0 | 435213.49 | 0.00E+00 | 300 | | PARAMETER | 2.74E+08 | 3.69E+03 |
| Carbon-14 | 162.3 | 2189.49 | 0.00E+00 | 2000 | | 1.62E+02 | 4.56E+01 | 1.24E+02 |
| Cesium-134 | 4032.7 | 54413.49 | 0.00E+00 | 80 | | PARAMETER | 3.05E+10 | 1.23E+02 |
| Cesium-137 | 4032.7 | 54413.49 | 0.00E+00 | 200 | | PARAMETER | 2.25E+01 | 3.08E+02 |
| Cobalt-57 | 81.6 | 1101.49 | 0.00E+00 | 1000 | | PARAMETER | 5.59E+29 | 3.14E+01 |
| Cobalt-60 | 81.6 | 1101.49 | 0.00E+00 | 100 | | 2.53E+63 | 2.25E+04 | 3.14E+00 |
| Curium-242 | 24997.8 | 337293.49 | 0.00E+00 | 15 | | PARAMETER | 4.59E+46 | 1.43E+02 |
| Curium-243/244 | 24997.8 | 337293.49 | 0.00E+00 | 15 | | PARAMETER | 1.86E+00 | 1.43E+02 |
| Curium-245/246 | 24997.8 | 337293.49 | 0.00E+00 | 15 | | 1.25E+14 | 3.41E-01 | 1.43E+02 |
| Curium-247 | 24997.8 | 337293.49 | 0.00E+00 | 15 | | 1.45E+02 | 3.39E-01 | 1.43E+02 |
| Europium-152 | 1976.6 | 26669.49 | 0.00E+00 | 60 | | PARAMETER | 4.80E+01 | 4.53E+01 |
| Europium-154 | 1976.6 | 26669.49 | 0.00E+00 | 200 | | PARAMETER | 1.12E+03 | 1.51E+02 |
| Europium-155 | 1976.6 | 26669.49 | 0.00E+00 | 600 | | PARAMETER | 2.40E+05 | 4.53E+02 |
| Iodine-129 | 30.0 | 405.17 | 0.00E+00 | 1.0 | | 1.17E-02 | 2.26E-02 | 1.17E-02 |
| Lead-212 | 2178.1 | 29389.49 | 0.00E+00 | 15 | | PARAMETER | PARAMETER | 1.25E+01 |
| Manganese-54 | 404.2 | 5453.49 | 0.00E+00 | 300 | | PARAMETER | 2.43E+25 | 4.63E+01 |
| Neptunium-237 | 81.6 | 1101.49 | 0.00E+00 | 15 | | 4.71E-01 | 3.39E-01 | 4.71E-01 |
| Neptunium-239 | 81.6 | 1101.49 | 0.00E+00 | 11.2 | | PARAMETER | PARAMETER | 3.52E-01 |
| Nickel-63 | 525.1 | 7085.49 | 0.00E+00 | 50 | | 2.12E+22 | 1.84E+00 | 1.00E+01 |
| Plutonium-238 | 807.3 | 10893.49 | 0.00E+00 | 15 | | 1.01E+38 | 5.89E-01 | 4.62E+00 |
| Plutonium-239/240 | 807.3 | 10893.49 | 0.00E+00 | 15 | | 6.32E+00 | 3.40E-01 | 4.62E+00 |
| Potassium-40 | 605.8 | 8173.49 | 0.00E+00 | NA | | PARAMETER | PARAMETER | PARAMETER |
| Promethium-147 | 1936.2 | 26125.49 | 0.00E+00 | 600 | | PARAMETER | 1.49E+09 | 4.43E+02 |
| Radium-226 | 807.3 | 10893.49 | 0.00E+00 | 5 | | 1.73E+02 | 1.17E-01 | 1.54E+00 |
| Radium-228 | 807.3 | 10893.49 | 0.00E+00 | 5 | | PARAMETER | 5.22E+02 | 1.54E+00 |
| Sodium-22 | 807.3 | 10893.49 | 0.00E+00 | 400 | | PARAMETER | 1.15E+09 | 1.23E+02 |
| Strontium-90 | 65.5 | 883.89 | 0.00E+00 | 8 | | 4.05E+08 | 9.87E-01 | 2.02E-01 |
| Technetium-99 | 1.8 | 24.37 | 1.04E+03 | 900 | | 8.67E-01 | 2.04E+01 | 8.67E-01 |
| Thorium-228 | 807.3 | 10893.49 | 0.00E+00 | 15 | | PARAMETER | 3.64E+10 | 4.62E+00 |
| Thorium-230 | 807.3 | 10893.49 | 0.00E+00 | 15 | | 5.10E+00 | 3.39E-01 | 4.62E+00 |
| Thorium-232 | 807.3 | 10893.49 | 0.00E+00 | 15 | | 4.62E+00 | 3.39E-01 | 4.62E+00 |
| Uranium-233/234 | 323.5 | 4365.49 | 0.00E+00 | 10 | | 1.25E+00 | 2.26E-01 | 1.24E+00 |
| Uranium-235 | 323.5 | 4365.49 | 0.00E+00 | 0.5 | | 6.18E-02 | 1.13E-02 | 6.18E-02 |
| Uranium-238 | 323.5 | 4365.49 | 0.00E+00 | 10 | | 1.24E+00 | 2.26E-01 | 1.24E+00 |
| Zinc-65 | 500.9 | 6759.09 | 0.00E+00 | 300 | | PARAMETER | 2.34E+32 | 5.74E+01 |
| Zirconium-95 | 4839.1 | 65293.49 | 0.00E+00 | 200 | | PARAMETER | 1.10E+121 | 3.69E+02 |

8/6/2004 12:39

PARAMETER indicates that a variable within the equation is not available such as the Kd or T1/2 or the source concentration has been decayed to zero.

*Uranium activities in water are calculated for the isotopic distribution of naturally occurring uranium. Total activity should not exceed 20.5 pCi/L.